

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
 Data File : BF139386.D
 Acq On : 16 Sep 2024 18:51
 Operator : RC/JU
 Sample : P3930-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DN-B-33

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139386.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	15	22	rVB	625503	953520	73.04%	9.081%
2	5.093	501	510	519	rBB	52197	78196	5.99%	0.745%
3	5.493	572	578	583	rBV	890683	1167958	89.46%	11.123%
4	6.504	743	750	755	rBV	874829	1203679	92.20%	11.463%
5	6.875	808	813	818	rBV	314491	378553	29.00%	3.605%
6	7.440	903	909	914	rBV	601294	778097	59.60%	7.410%
7	7.692	948	952	956	rBB	19918	23732	1.82%	0.226%
8	8.157	1026	1031	1036	rBV	382330	459709	35.21%	4.378%
9	9.234	1208	1214	1219	rBV	1063817	1305519	100.00%	12.433%
10	9.910	1324	1329	1334	rBV	364473	434962	33.32%	4.142%
11	10.622	1445	1450	1456	rBV	78719	93327	7.15%	0.889%
12	10.692	1457	1462	1473	rVB	505077	649163	49.72%	6.182%
13	11.392	1576	1581	1589	rVB	307581	380880	29.17%	3.627%
14	11.916	1663	1670	1682	rBV	146401	217202	16.64%	2.068%
15	12.604	1782	1787	1799	rBV	21915	41899	3.21%	0.399%
16	12.698	1799	1803	1810	rBV	20722	32073	2.46%	0.305%
17	12.827	1822	1825	1831	rVB	13959	17891	1.37%	0.170%
18	12.974	1845	1850	1857	rVB	741285	940094	72.01%	8.953%
19	13.451	1923	1931	1937	rBV	33083	54631	4.18%	0.520%
20	13.874	1998	2003	2019	rBV	53194	113639	8.70%	1.082%
21	14.027	2022	2029	2037	rVB	221287	314610	24.10%	2.996%
22	14.316	2074	2078	2083	rBV3	10672	13728	1.05%	0.131%
23	14.504	2105	2110	2123	rBV3	28039	77688	5.95%	0.740%
24	14.880	2170	2174	2181	rVB	29272	40520	3.10%	0.386%
25	14.951	2182	2186	2192	rBV4	17800	27616	2.12%	0.263%
26	15.068	2202	2206	2214	rVB2	8530	17968	1.38%	0.171%
27	15.145	2214	2219	2223	rBV	46785	68253	5.23%	0.650%
28	15.498	2273	2279	2289	rVB	125056	204461	15.66%	1.947%
29	15.733	2314	2319	2328	rVB2	18913	35290	2.70%	0.336%
30	15.968	2354	2359	2365	rBV	36984	61765	4.73%	0.588%
31	16.774	2491	2496	2505	rVB7	11350	24177	1.85%	0.230%
32	17.145	2552	2559	2568	rBV	101642	209013	16.01%	1.991%
33	17.480	2611	2616	2623	rVB5	14034	30017	2.30%	0.286%
34	17.980	2694	2701	2707	rVB9	10697	28295	2.17%	0.269%
35	18.592	2800	2805	2818	rVB9	6352	22359	1.71%	0.213%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

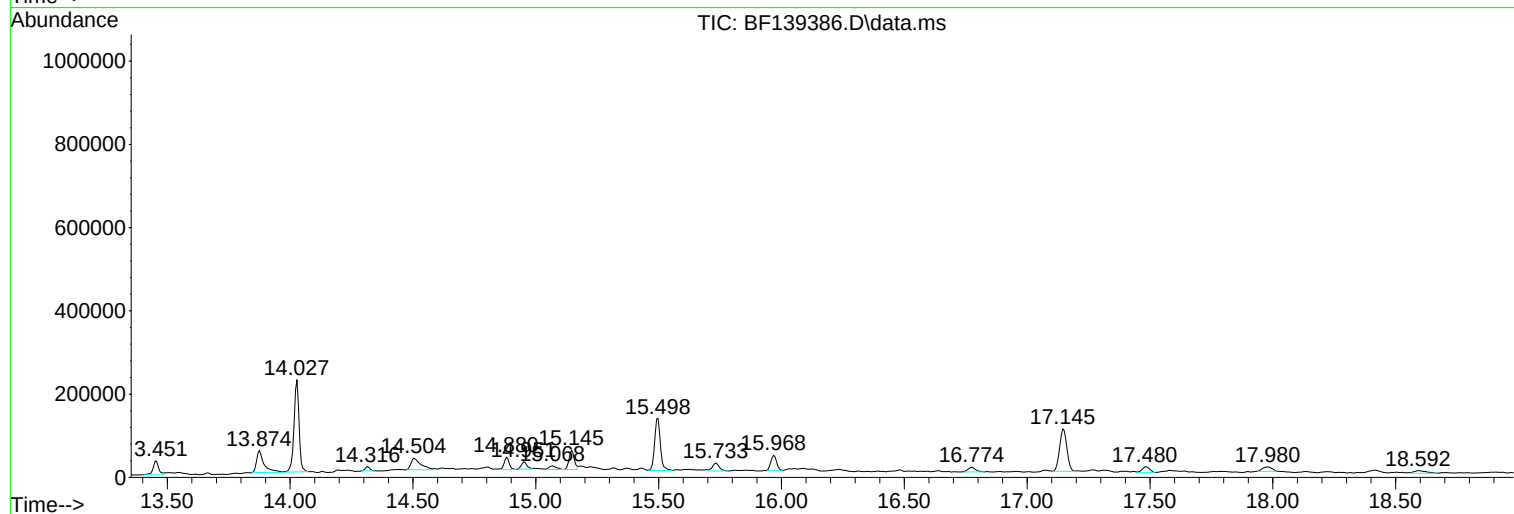
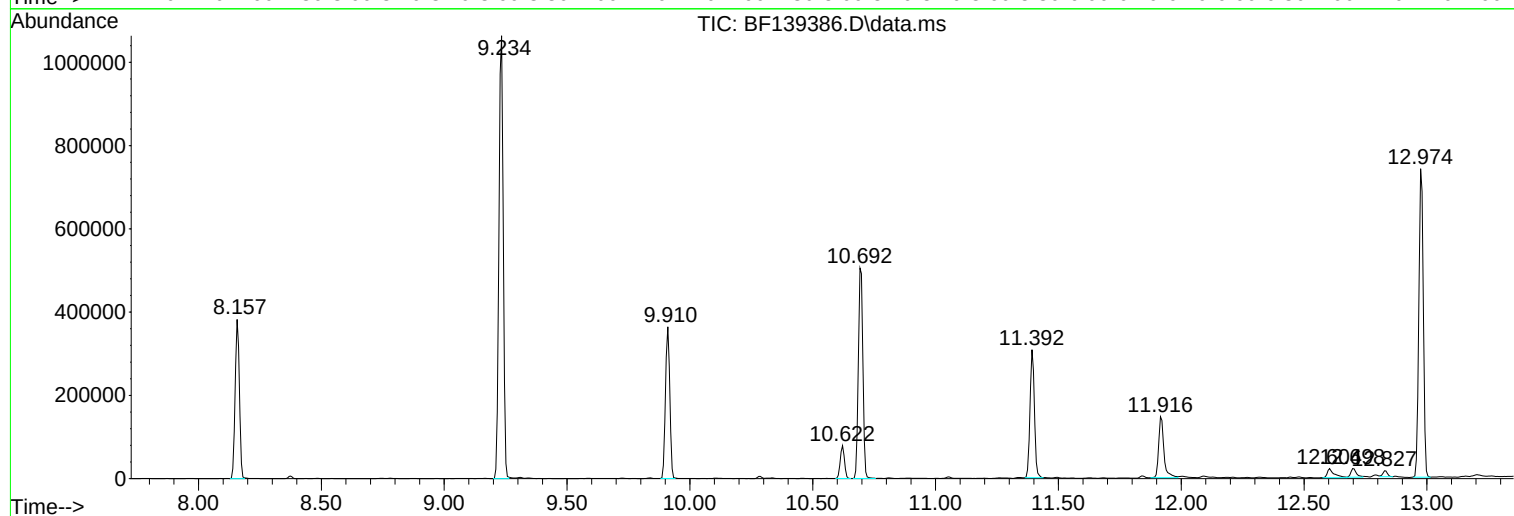
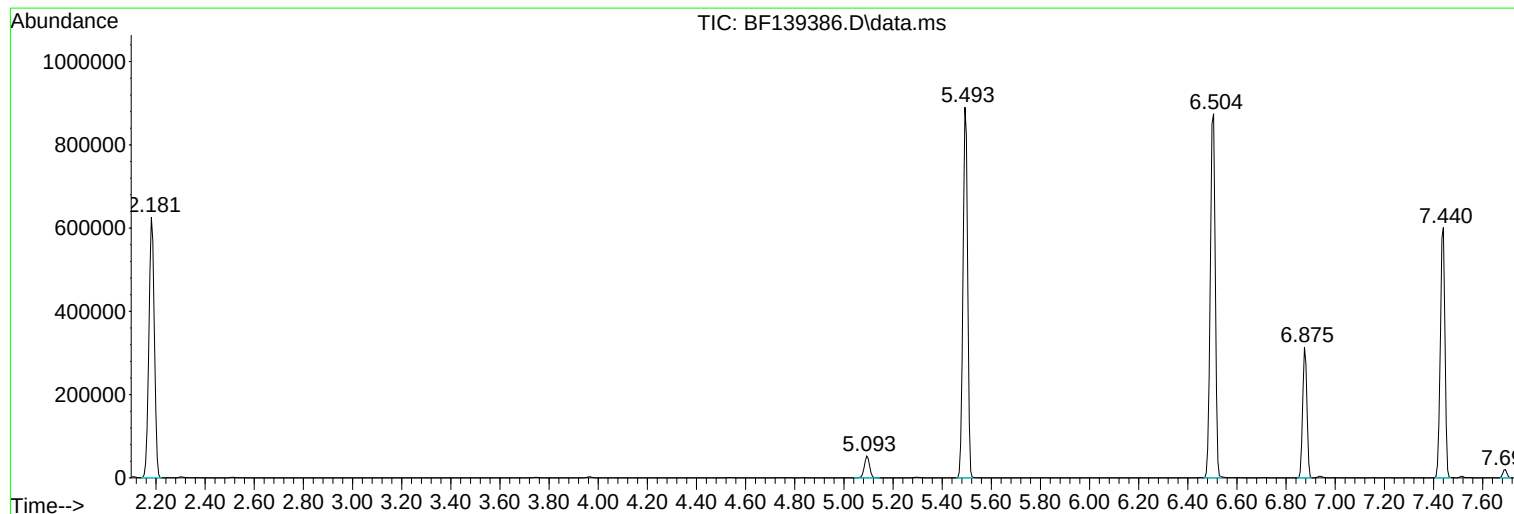
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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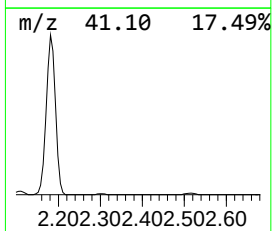
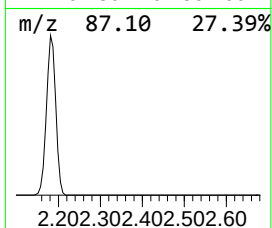
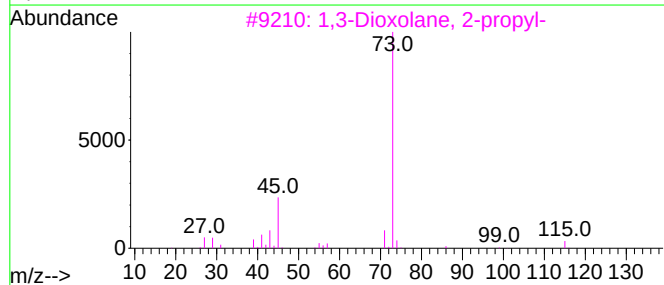
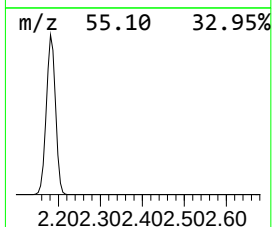
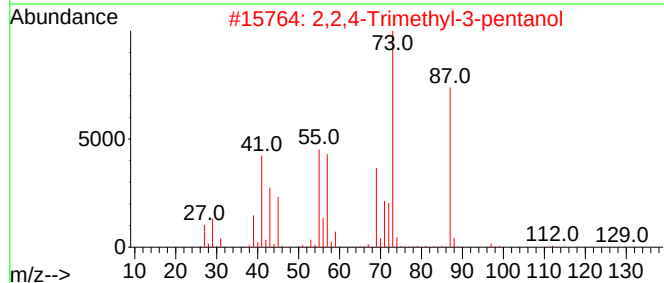
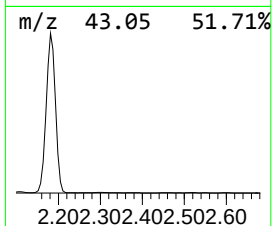
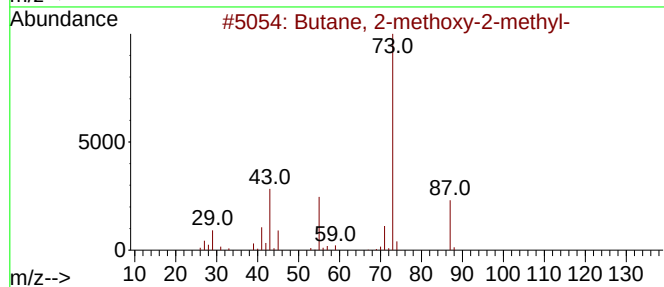
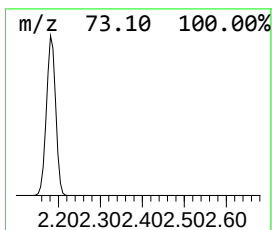
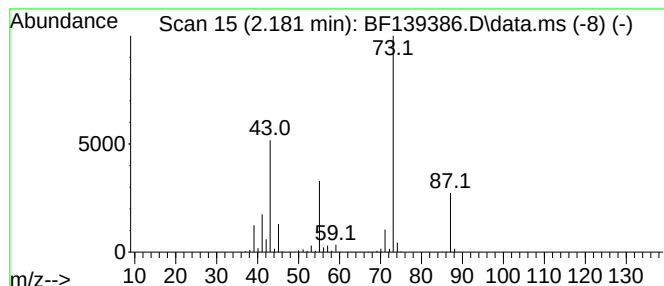
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	50.38 ng	953520	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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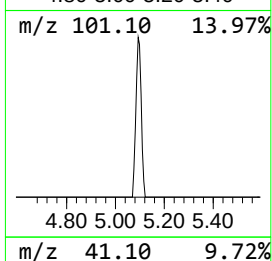
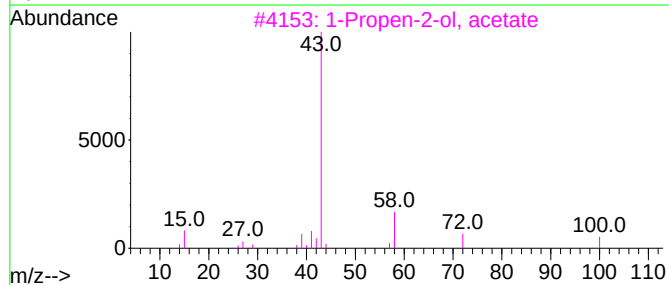
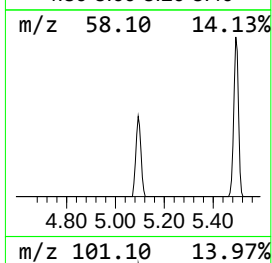
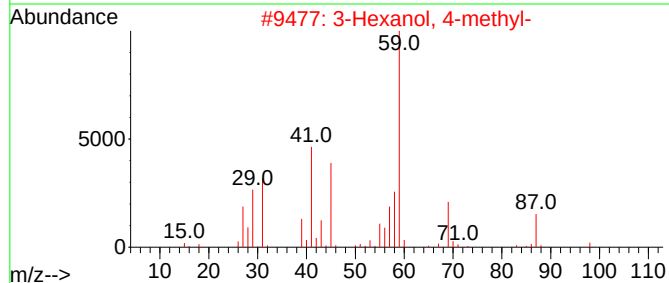
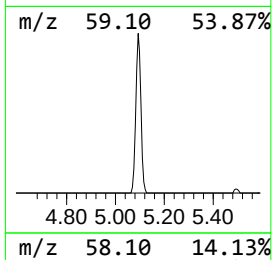
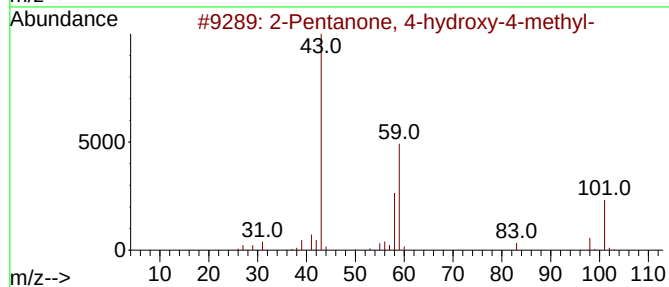
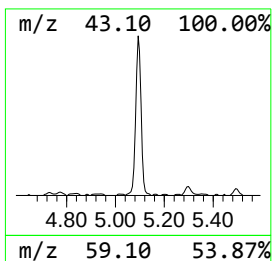
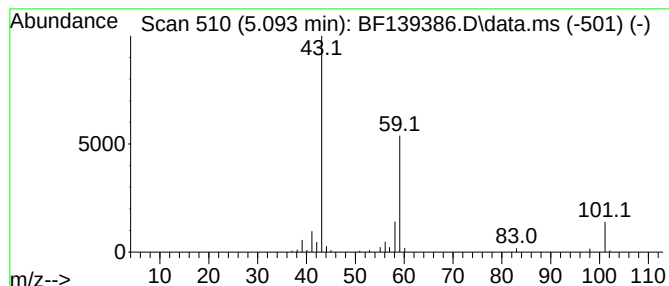
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	4.13 ng	78196	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane	58	C4H10	000106-97-8	9



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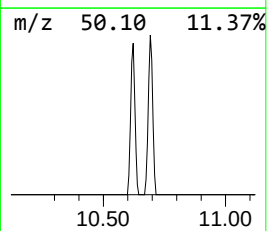
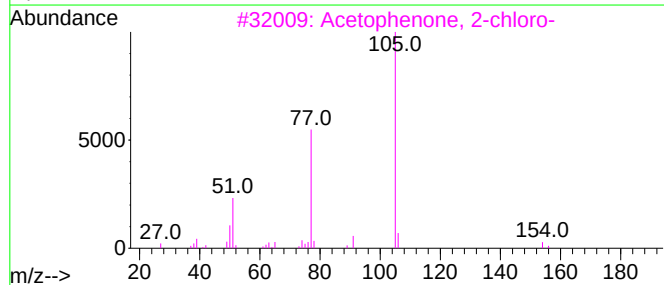
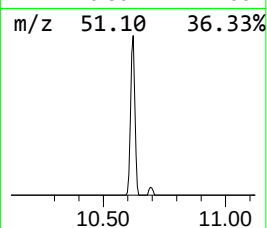
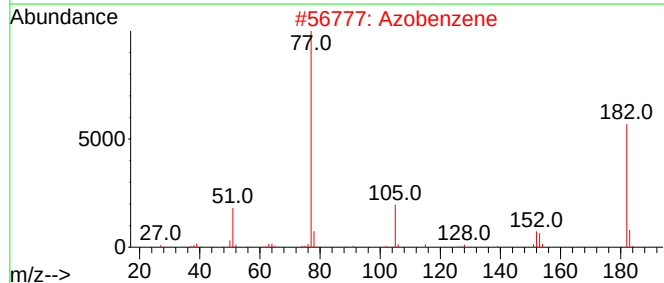
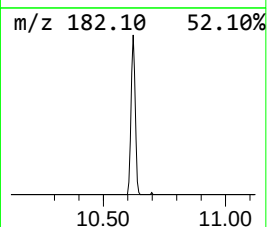
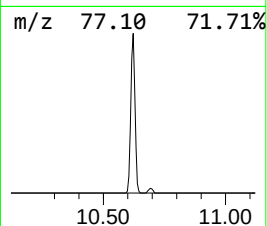
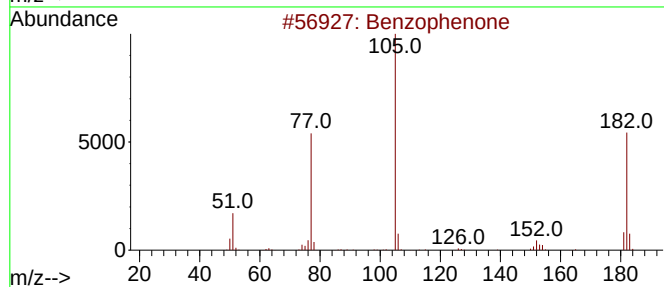
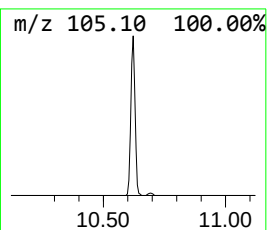
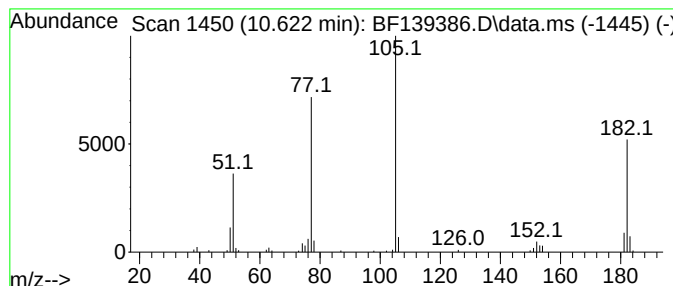
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	4.29 ng	93327	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	50



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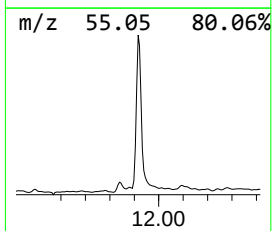
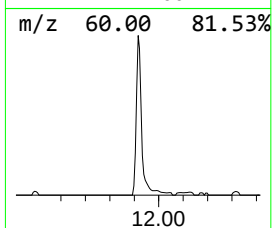
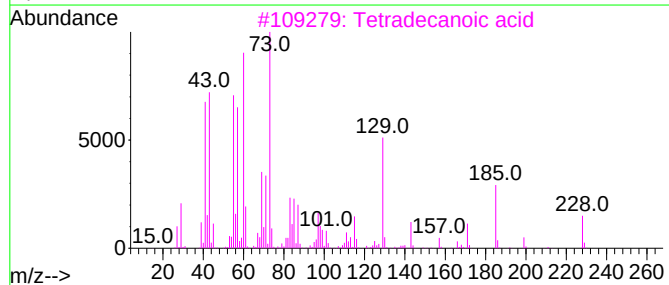
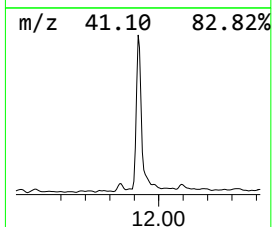
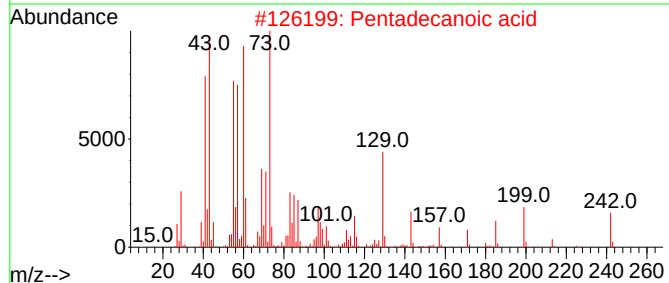
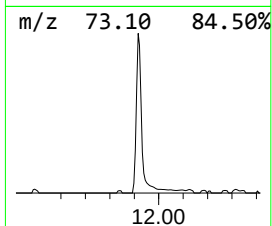
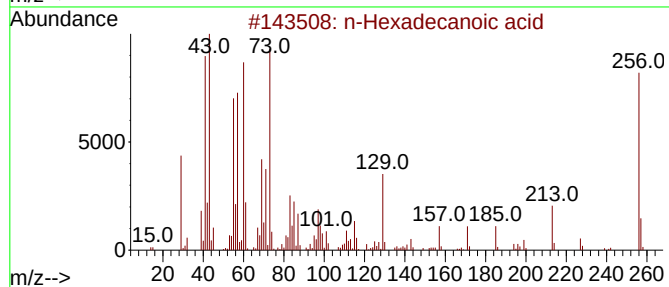
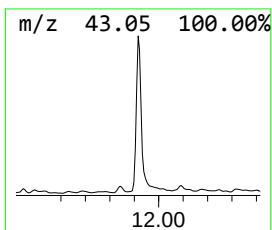
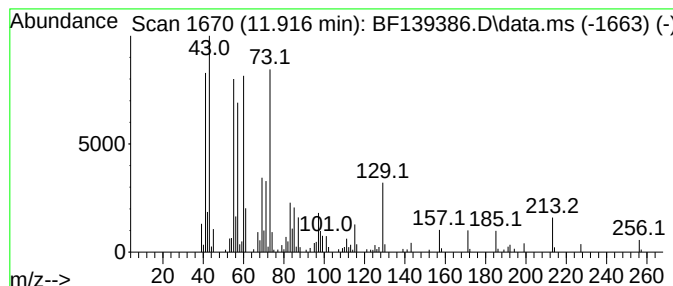
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	11.41 ng	217202	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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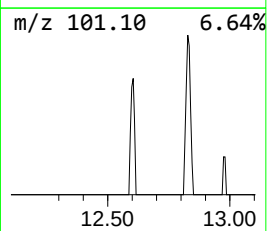
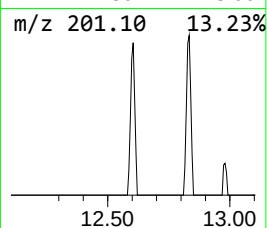
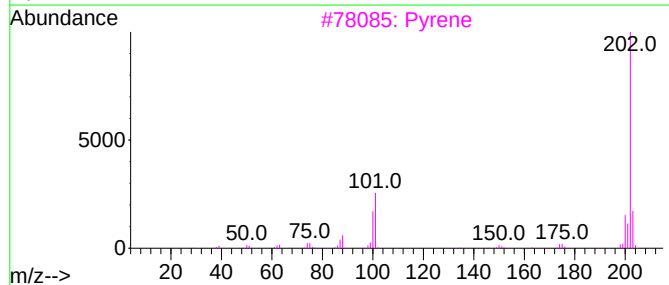
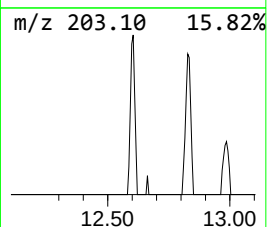
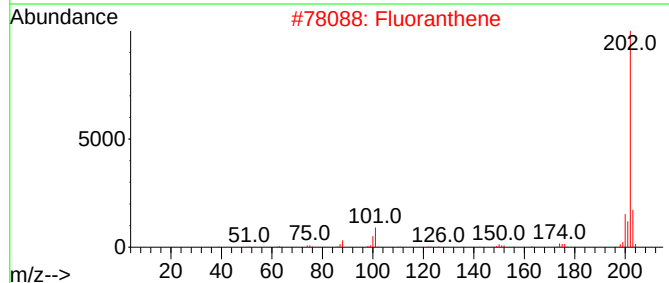
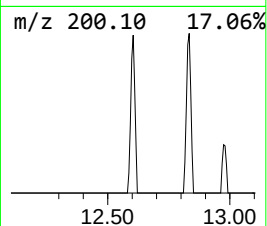
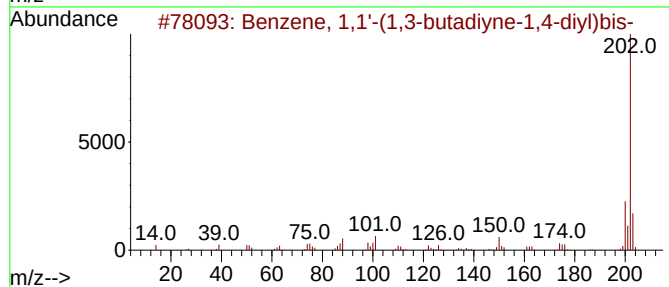
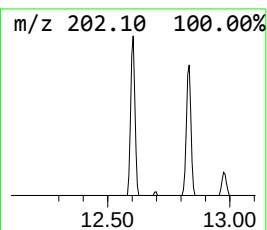
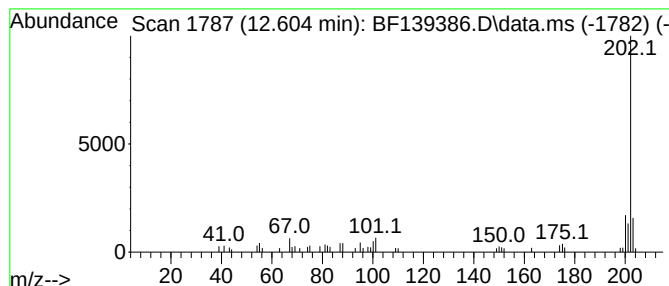
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	2.20 ng	41899	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	90
2			Fluoranthene	202	C16H10	000206-44-0	83
3			Pyrene	202	C16H10	000129-00-0	76
4			5-(4-Methylphenyl)furan-2-carbox...	202	C12H10O3	1000305-27-5	53
5			7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

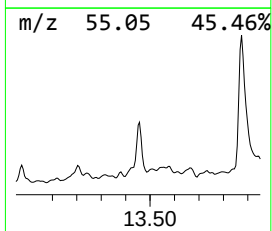
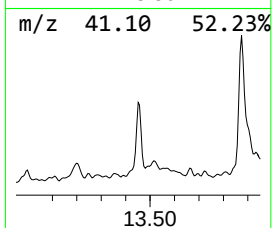
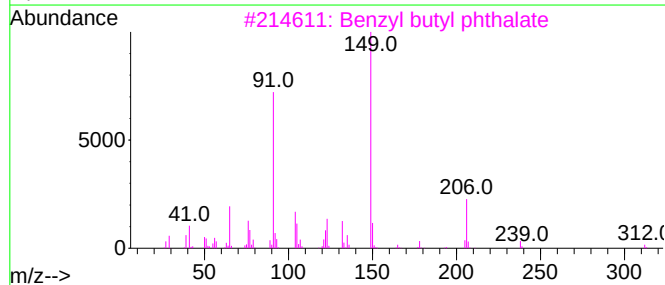
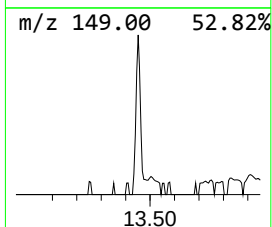
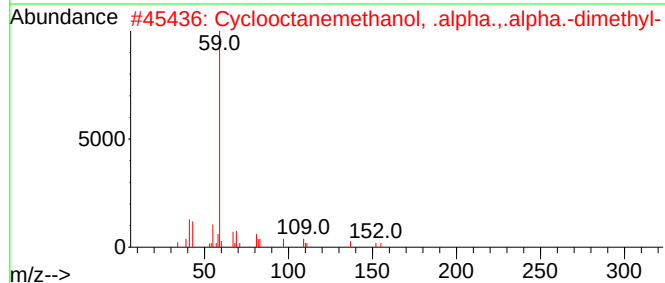
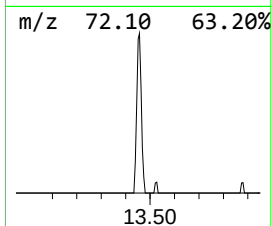
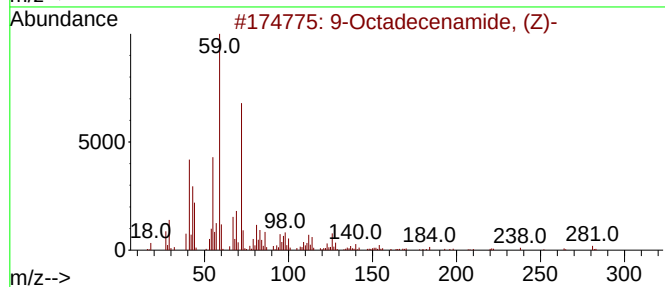
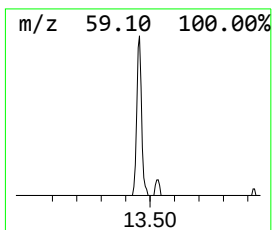
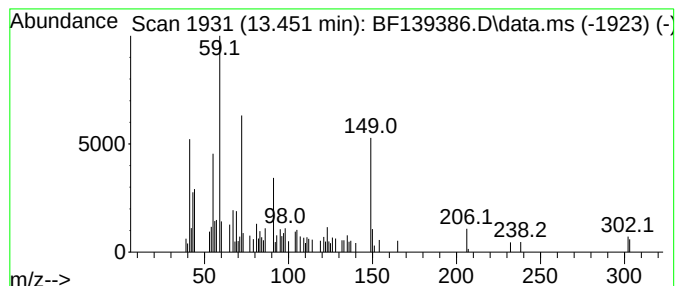
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ClientSampleId :
DN-B-33

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown13.451 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.451	3.47 ng	54631	Chrysene-d12	14.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	49
2	Cyclooctanemethanol, .alpha.,.al...	170	C11H22O	016624-06-9	25
3	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	22
4	Phthalic acid, 3-methylbenzyl is...	326	C20H22O4	1010371-10-7	14
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
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Sample : P3930-01
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Instrument :
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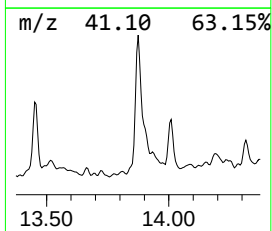
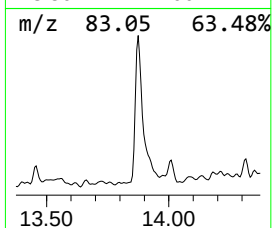
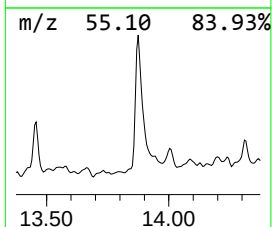
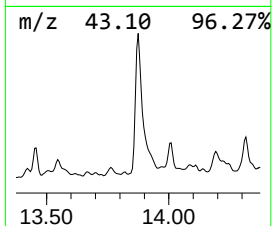
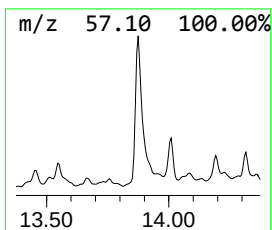
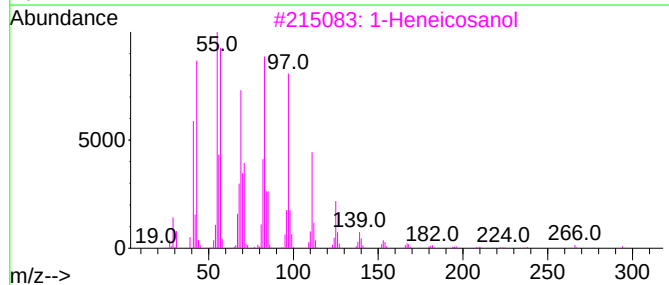
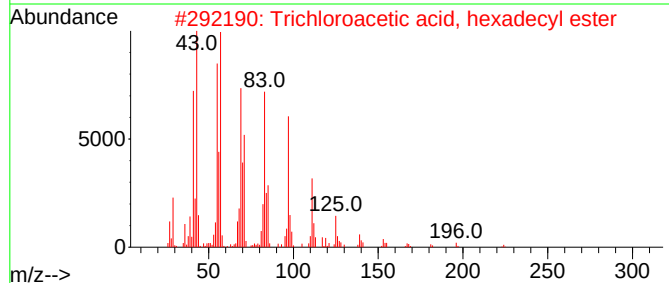
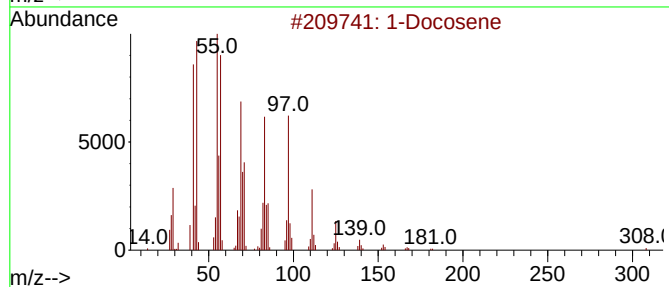
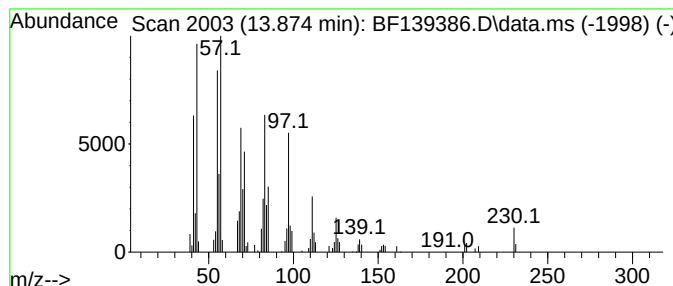
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	7.22 ng	113639	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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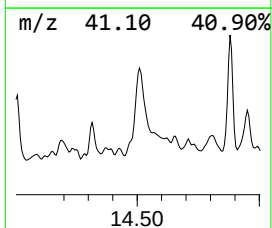
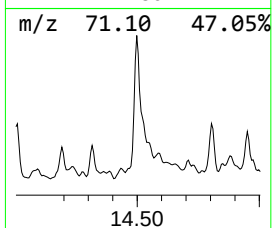
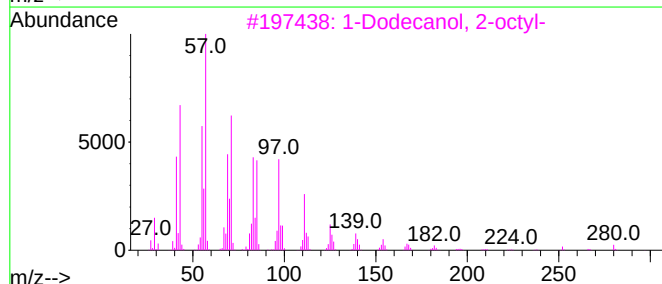
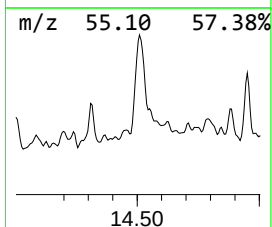
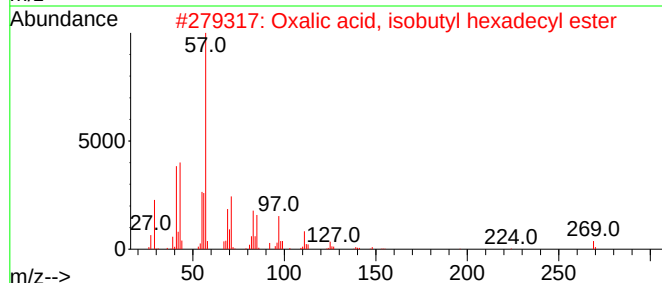
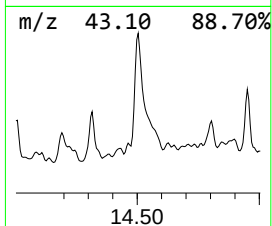
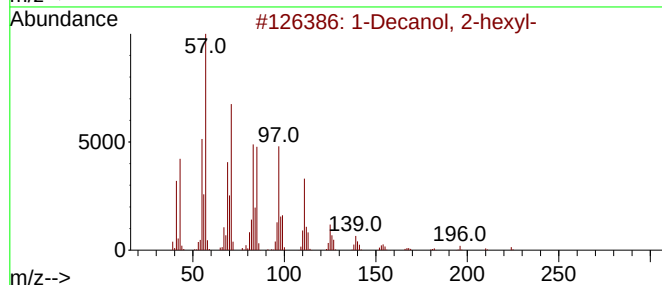
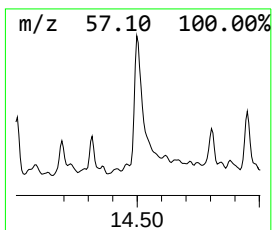
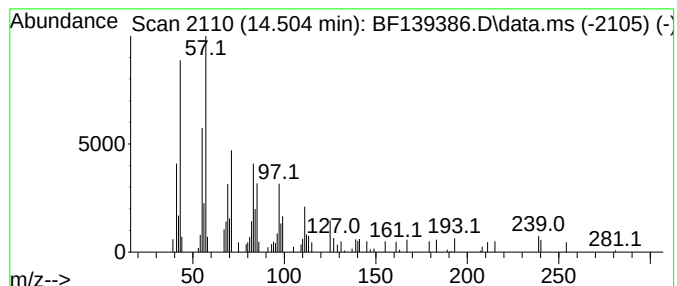
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	4.94 ng	77688	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
3			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
4			Isobutyl tetratriacontyl ether	551	C38H78O	1000406-33-7	83
5			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
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Instrument :
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ClientSampleId :
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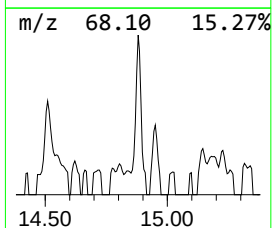
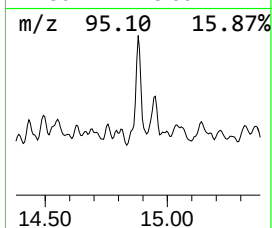
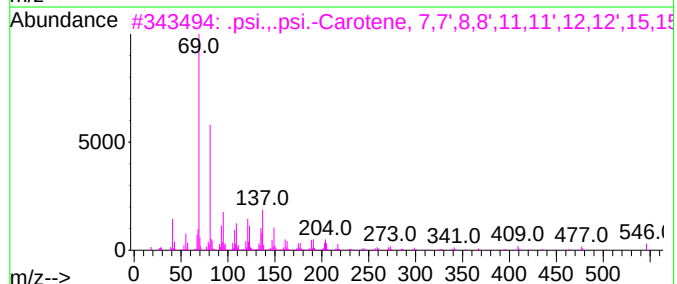
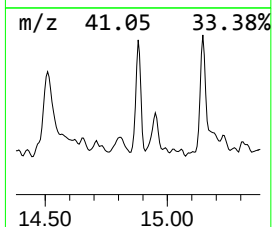
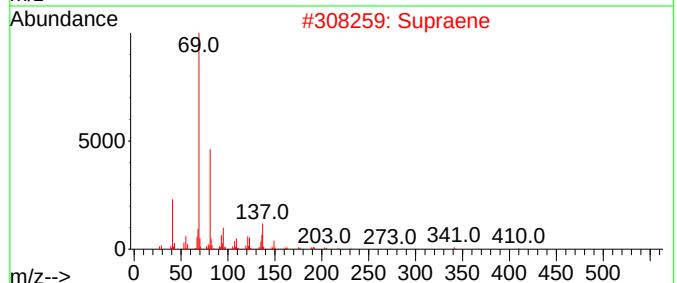
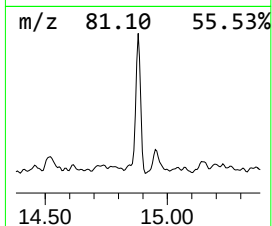
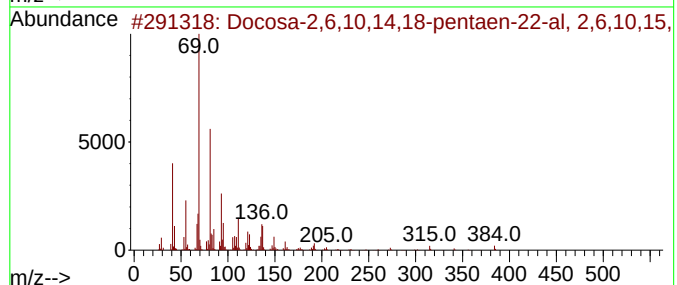
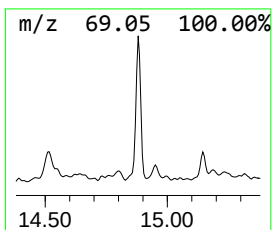
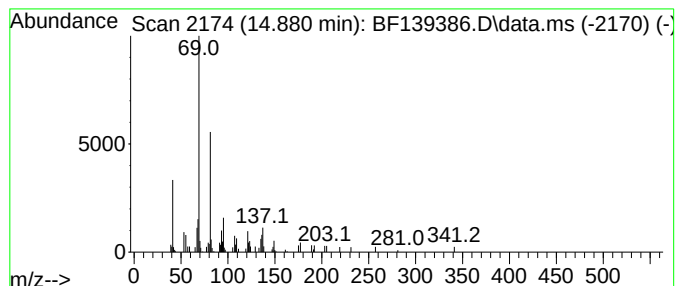
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	3.96 ng	40520	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2			Supraene	410	C30H50	007683-64-9	87
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
5			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
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Instrument :
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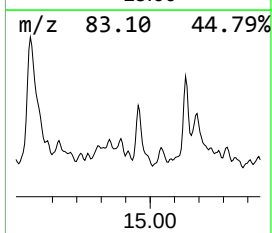
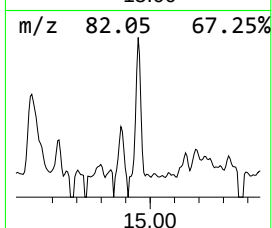
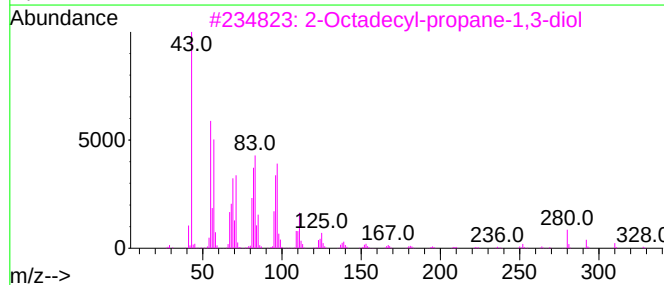
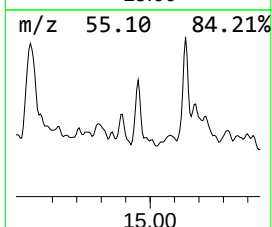
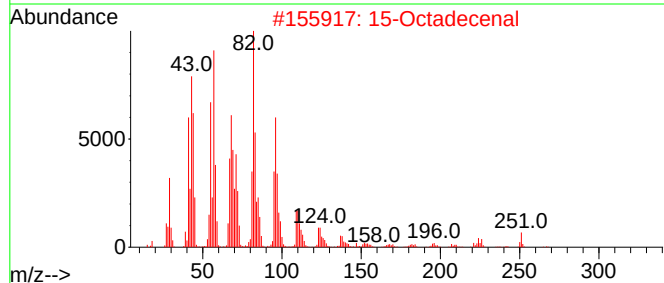
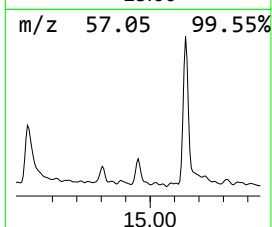
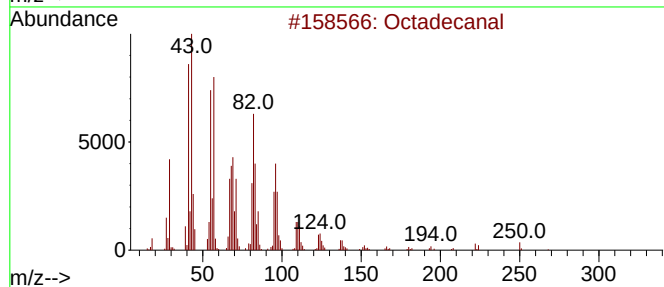
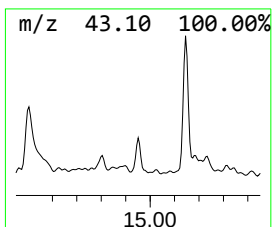
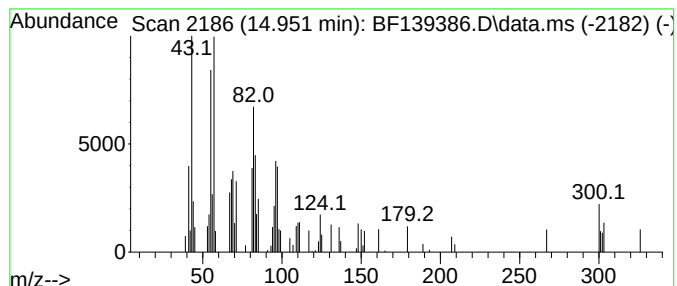
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	2.70 ng	27616	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	64
2			15-Octadecenal	266	C18H34O	056554-93-9	52
3			2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	52
4			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	52
5			1,19-Eicosadiene	278	C20H38	014811-95-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
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Sample : P3930-01
Misc :
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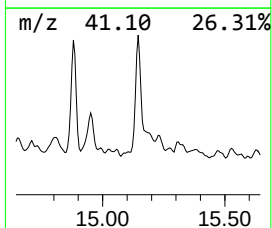
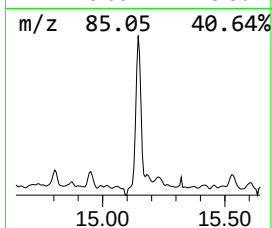
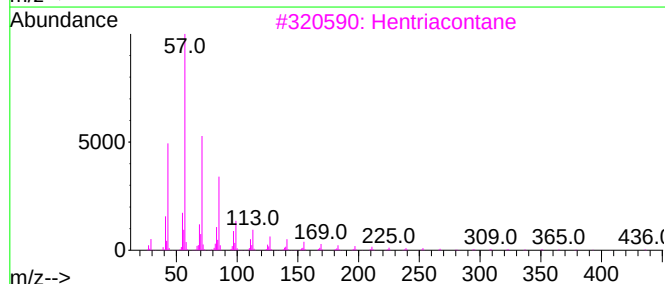
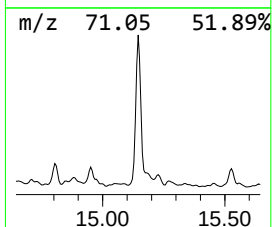
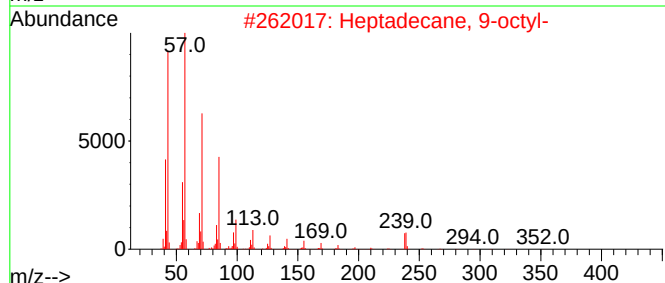
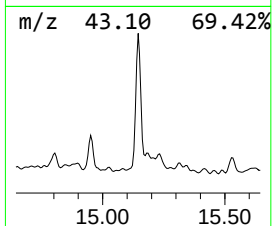
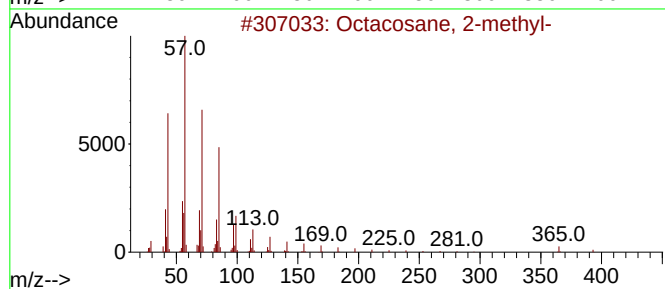
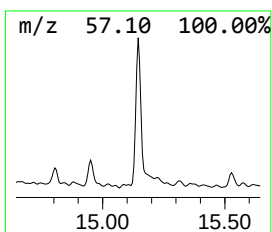
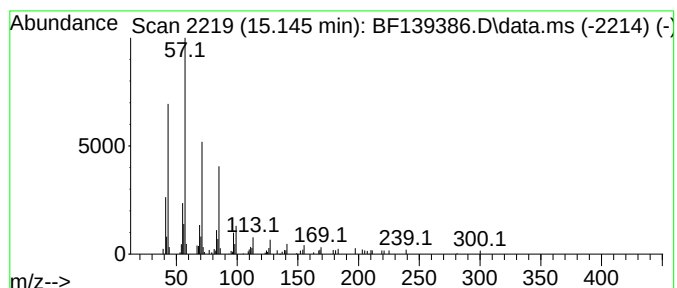
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	6.68 ng	68253	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
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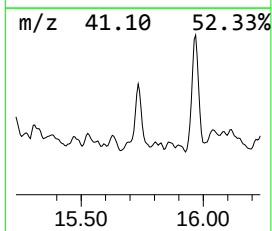
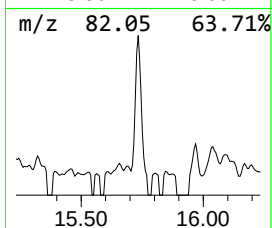
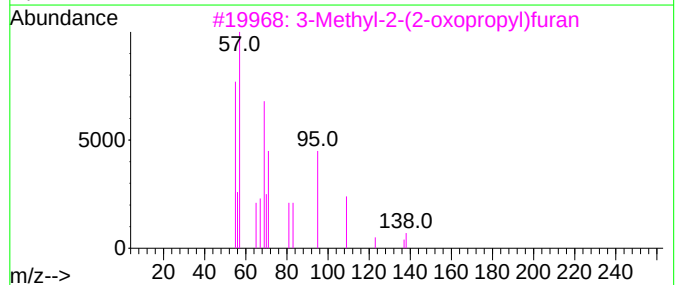
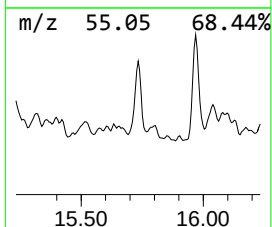
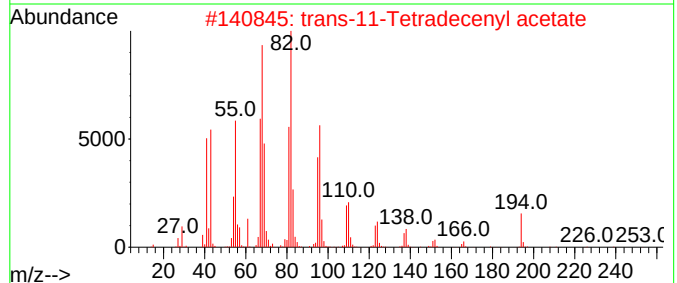
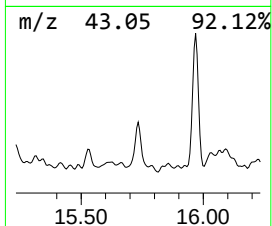
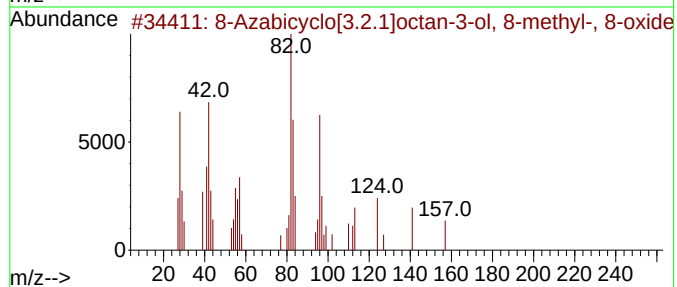
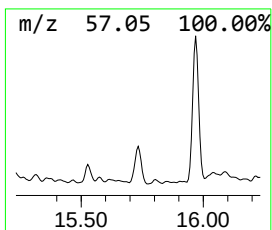
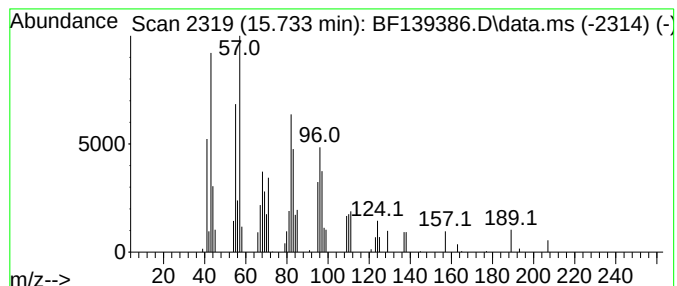
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 8-Azabicyclo[3.2.1]octan-3-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	3.45 ng	35290	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Azabicyclo[3.2.1]octan-3-ol, 8...	157	C8H15NO2	032663-71-1	64
2			trans-11-Tetradecenyl acetate	254	C16H30O2	033189-72-9	47
3			3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	45
4			Heptacosyl acetate	438	C29H58O2	1000351-78-2	43
5			Cyclododecanol	184	C12H24O	001724-39-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-33

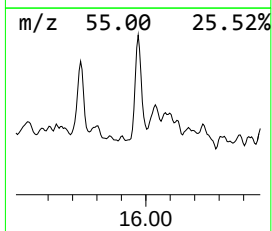
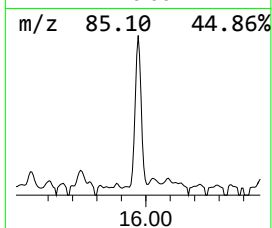
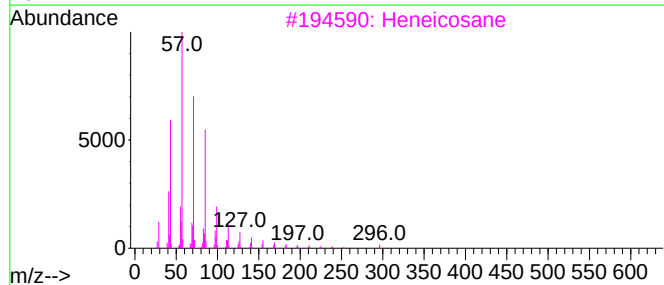
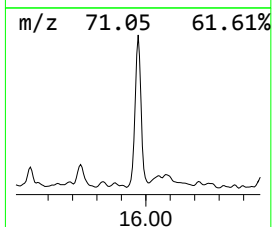
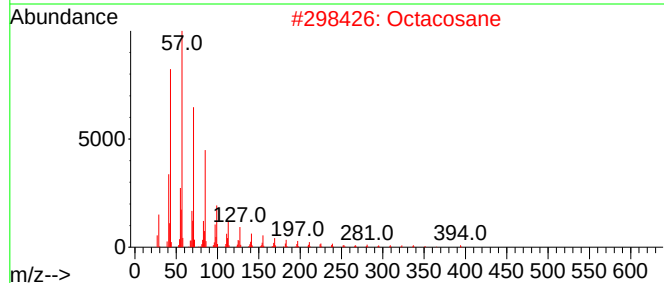
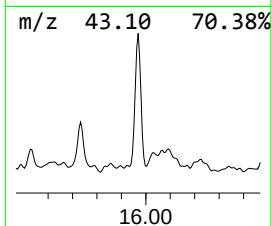
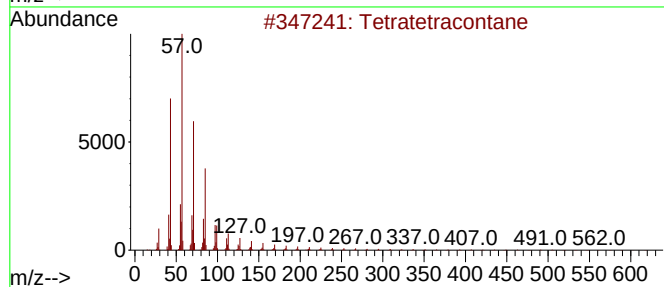
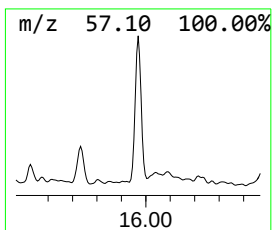
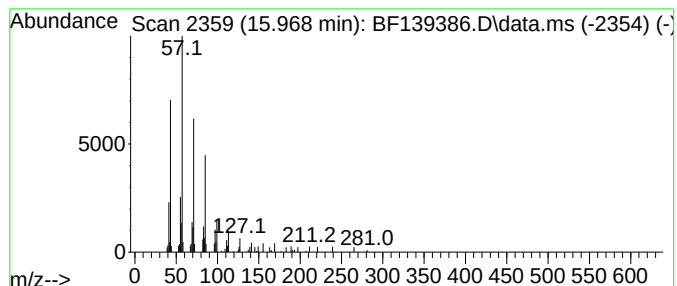
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	6.04 ng	61765	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
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Sample : P3930-01
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ClientSampleId :
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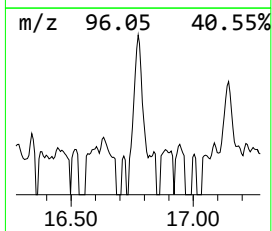
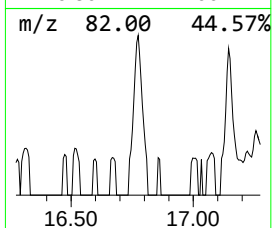
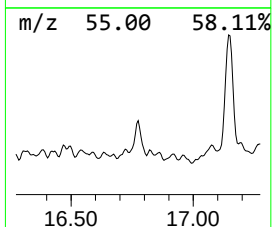
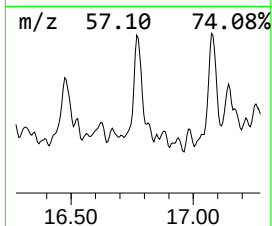
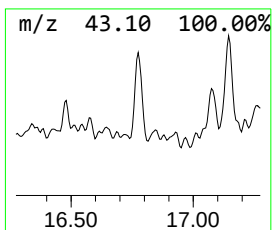
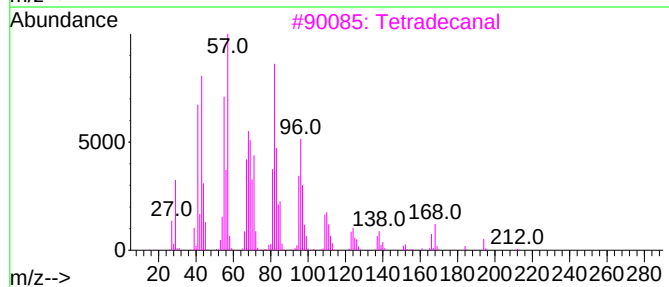
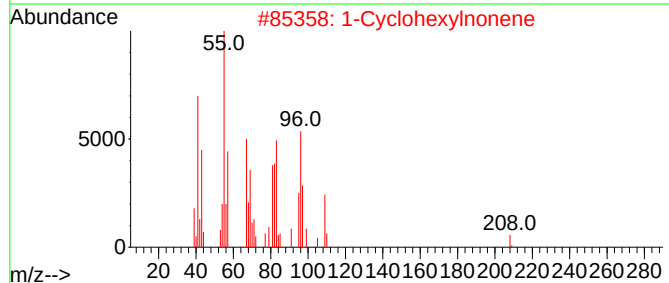
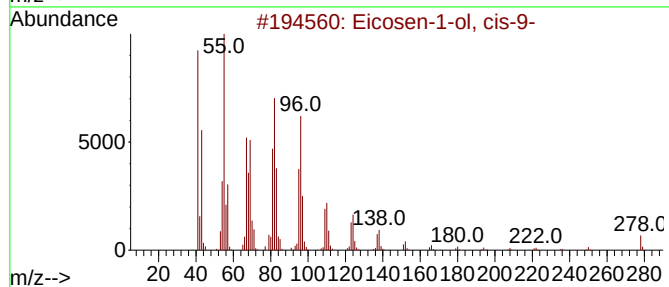
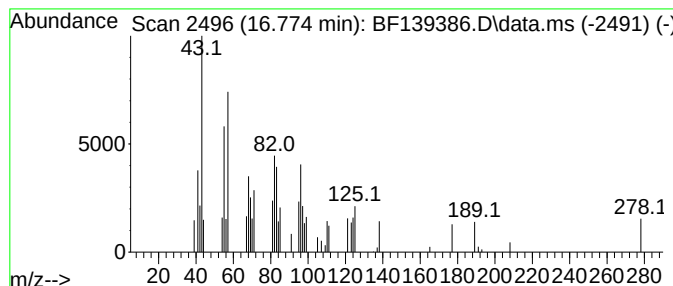
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Eicosen-1-ol, cis-9- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	2.36 ng	24177	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosen-1-ol, cis-9-	296	C20H40O	112248-30-3	50
2		1-Cyclohexylnonene	208	C15H28	114614-84-5	49
3		Tetradecanal	212	C14H28O	000124-25-4	47
4		3-Methoxy-2(1H)-pyridone	125	C6H7NO2	020928-63-6	38
5		Hexadecanal	240	C16H32O	000629-80-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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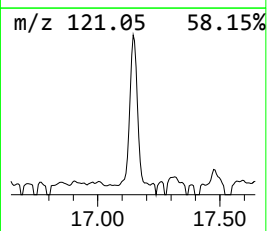
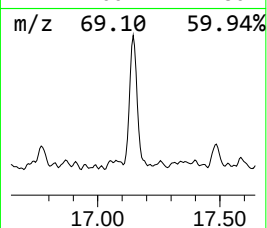
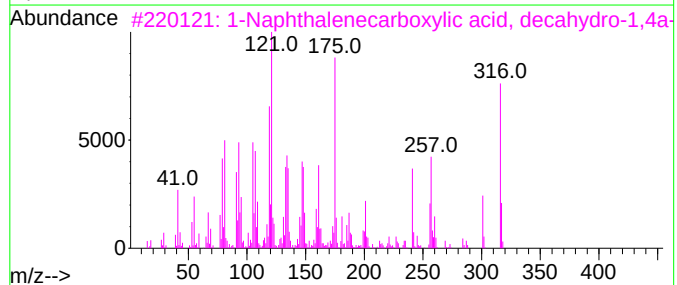
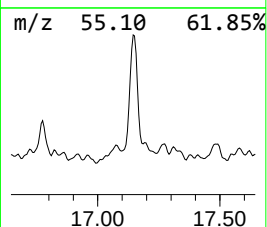
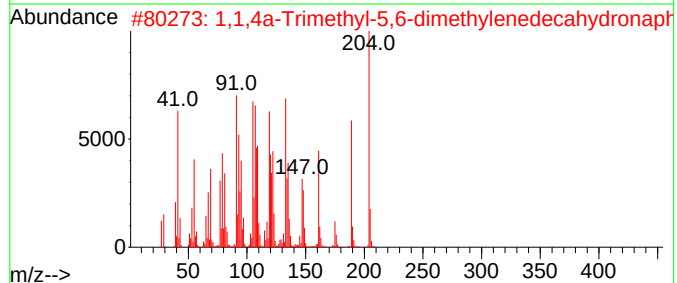
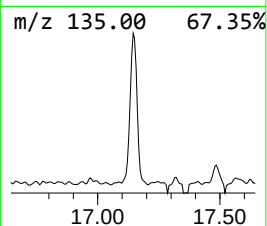
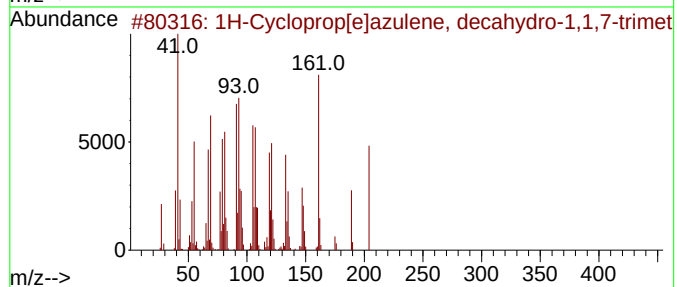
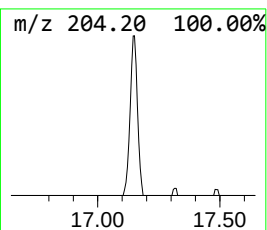
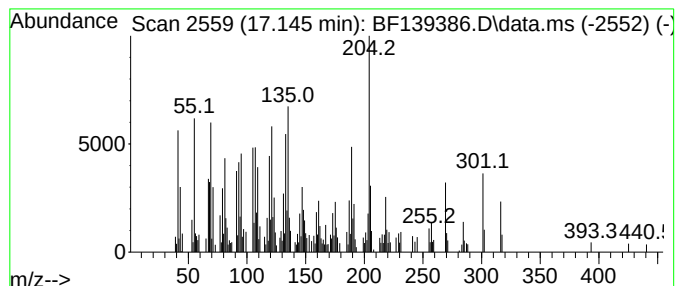
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1H-Cycloprop[e]azulene, dec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	20.45 ng	209013	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	83
2			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	83
3			1-Naphthalenecarboxylic acid, de...	316	C21H32O2	015798-13-7	68
4			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	64
5			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
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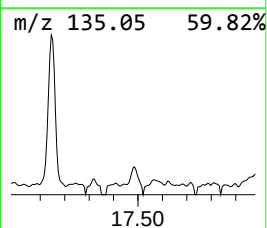
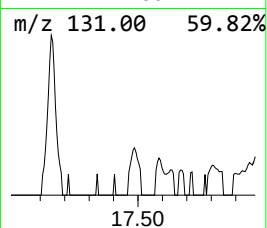
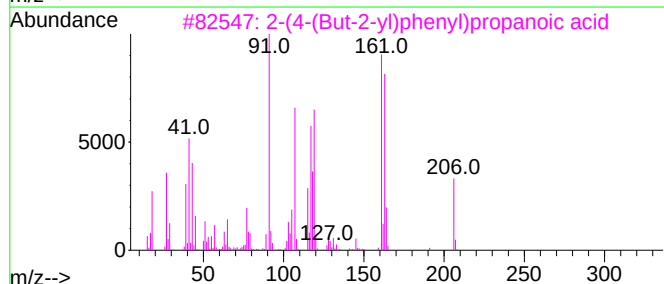
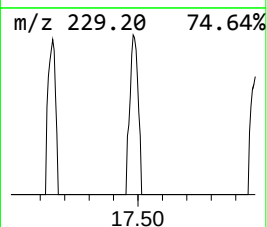
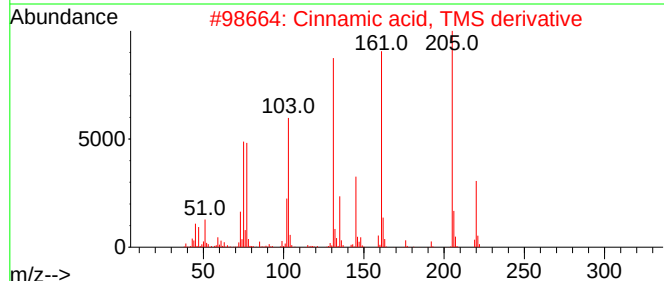
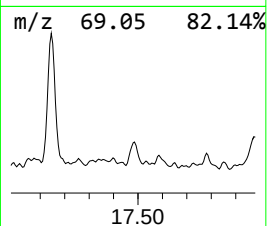
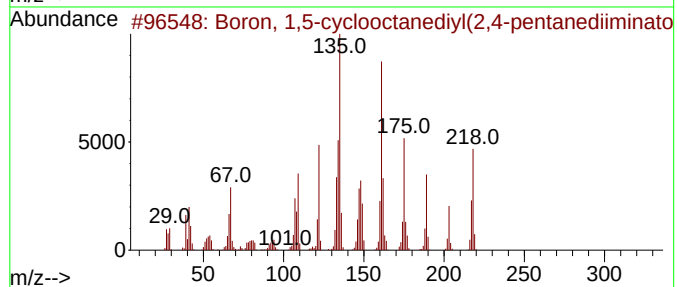
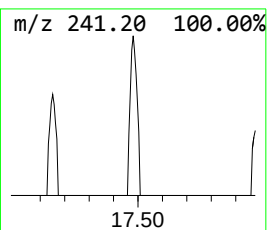
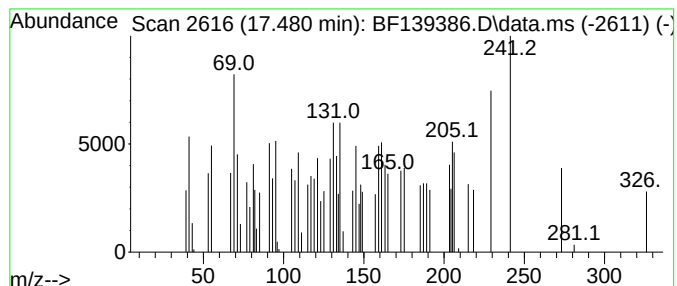
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BNA_F
ClientSampleId :
DN-B-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown17.480 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.480	2.94 ng	30017	Perylene-d12	15.498		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Boron, 1,5-cyclooctanediyl(2,4-p...	218	C13H23BN2	136704-99-9	15
2		Cinnamic acid, TMS derivative	220	C12H16O2Si	002078-20-8	10
3		2-(4-(But-2-yl)phenyl)propanoic ...	206	C13H18O2	064451-76-9	10
4		Silane, monochloride, methylviny...	218	C10H19ClOSi	1000421-09-7	10
5		Silane, monochloride, methylviny...	218	C10H19ClOSi	1000421-06-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
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Sample : P3930-01
Misc :
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Instrument :
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ClientSampleId :
DN-B-33

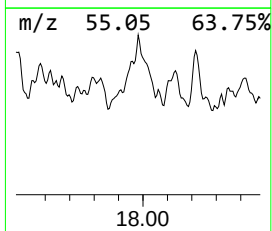
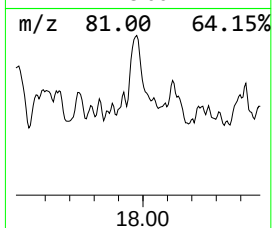
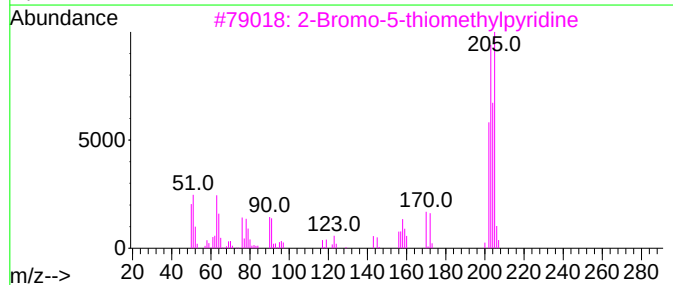
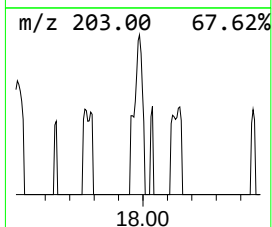
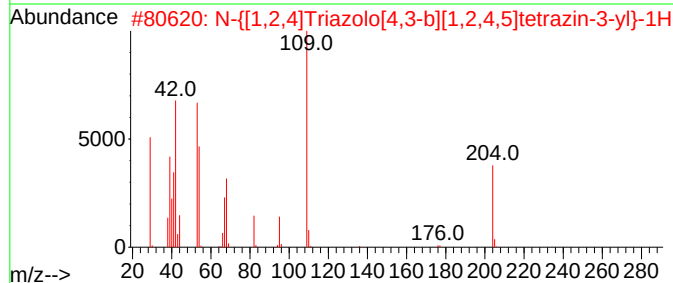
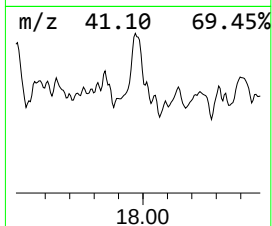
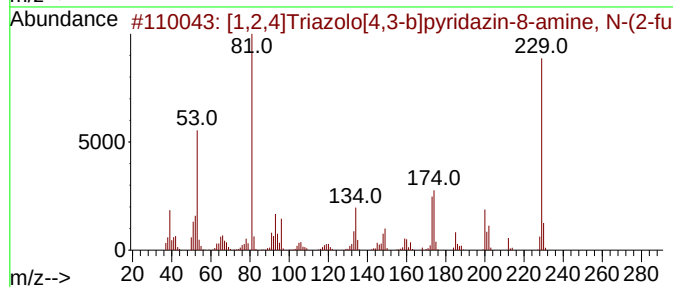
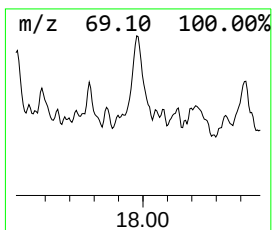
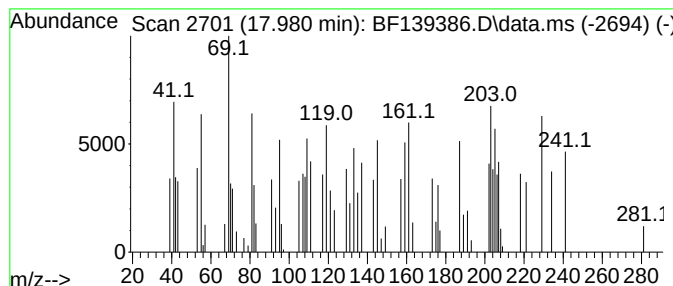
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown17.980 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	2.77 ng	28295	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,2,4]Triazolo[4,3-b]pyridazin-...	229	C11H11N5O	1000338-08-6	30
2			N-([1,2,4]Triazolo[4,3-b][1,2,4,...	204	C5H4N10	1000444-34-9	27
3			2-Bromo-5-thiomethylpyridine	203	C6H6BrNS	1000306-86-8	22
4			1H-Pyrazolo[4,3-d]pyrimidin-7-am...	203	C10H13N5	034232-31-0	22
5			2-Furanmethanamine, N-methyl-	111	C6H9NO	004753-75-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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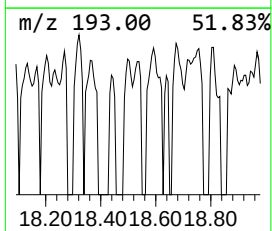
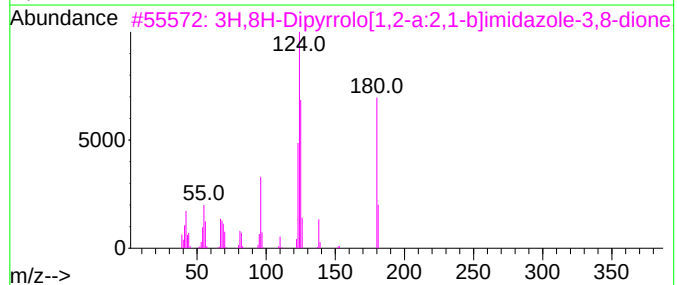
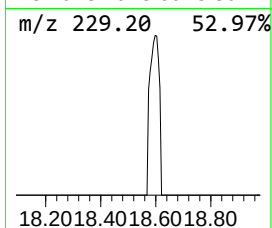
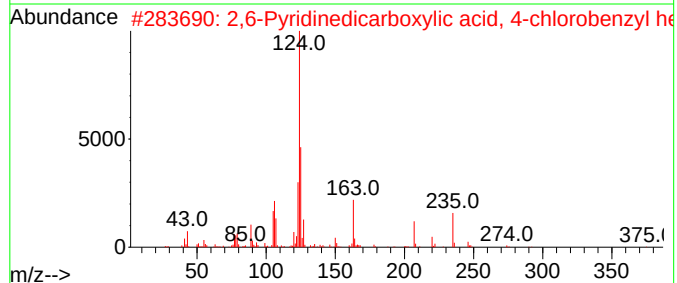
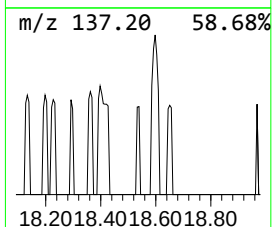
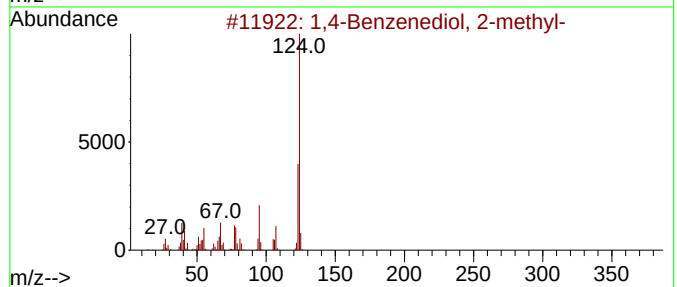
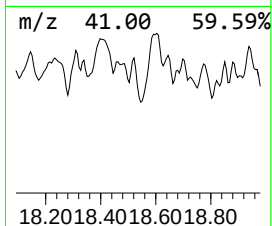
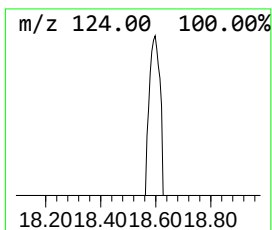
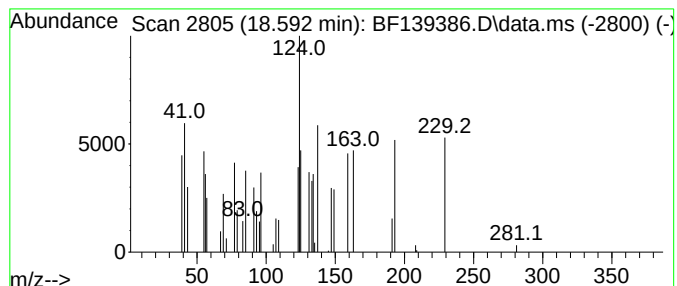
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown18.592 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.592	2.19 ng	22359	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	18
2			2,6-Pyridinedicarboxylic acid, 4...	375	C20H22ClNO4	1010369-14-1	17
3			3H,8H-Dipyrrolo[1,2-a:2,1-b]imid...	180	C9H12N2O2	040833-06-5	16
4			1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	14
5			Benzenemethanamine, 3-fluoro-	125	C7H8FN	000100-82-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139386.D
Acq On : 16 Sep 2024 18:51
Operator : RC/JU
Sample : P3930-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DN-B-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	50.4	ng	953520	1	6.875	378553	20.0
2-Pentanone, 4-...	5.093	4.1	ng	78196	1	6.875	378553	20.0
Benzophenone	10.622	4.3	ng	93327	3	9.910	434962	20.0
n-Hexadecanoic ...	11.916	11.4	ng	217202	4	11.392	380880	20.0
Benzene, 1,1'-(...	12.604	2.2	ng	41899	4	11.392	380880	20.0
unknown13.451	13.451	3.5	ng	54631	5	14.027	314610	20.0
1-Docosene	13.874	7.2	ng	113639	5	14.027	314610	20.0
1-Decanol, 2-he...	14.504	4.9	ng	77688	5	14.027	314610	20.0
Docosa-2,6,10,1...	14.880	4.0	ng	40520	6	15.498	204461	20.0
Octadecanal	14.951	2.7	ng	27616	6	15.498	204461	20.0
Octacosane, 2-m...	15.145	6.7	ng	68253	6	15.498	204461	20.0
8-Azabicyclo[3....	15.733	3.5	ng	35290	6	15.498	204461	20.0
Tetratetracontane	15.968	6.0	ng	61765	6	15.498	204461	20.0
Eicosen-1-ol, c...	16.774	2.4	ng	24177	6	15.498	204461	20.0
1H-Cycloprop[e]...	17.145	20.4	ng	209013	6	15.498	204461	20.0
unknown17.480	17.480	2.9	ng	30017	6	15.498	204461	20.0
unknown17.980	17.980	2.8	ng	28295	6	15.498	204461	20.0
unknown18.592	18.592	2.2	ng	22359	6	15.498	204461	20.0