

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
 Data File : BF139423.D
 Acq On : 18 Sep 2024 13:21
 Operator : RC/JU
 Sample : P4015-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-2-TANK17

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: BF139423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	9	18	32	rVB	806249	1286701	69.23%	8.011%
2	5.098	501	511	519	rBV	70203	107281	5.77%	0.668%
3	5.498	573	579	584	rBV	1155297	1502255	80.83%	9.353%
4	6.504	744	750	755	rBV	1166490	1585232	85.30%	9.869%
5	6.875	808	813	818	rVB	363128	451574	24.30%	2.811%
6	7.439	902	909	914	rBV	795404	1035824	55.73%	6.449%
7	7.692	948	952	956	rVB	20467	25045	1.35%	0.156%
8	8.157	1026	1031	1040	rBV	465284	585322	31.49%	3.644%
9	9.233	1208	1214	1219	rBV	1486601	1858489	100.00%	11.571%
10	9.910	1324	1329	1333	rBV	522026	649930	34.97%	4.046%
11	9.939	1333	1334	1339	rVB	54800	52653	2.83%	0.328%
12	10.110	1359	1363	1368	rVB	21199	27570	1.48%	0.172%
13	10.457	1418	1422	1426	rBV	37886	45288	2.44%	0.282%
14	10.622	1445	1450	1457	rVB	86740	108818	5.86%	0.677%
15	10.698	1457	1463	1468	rBV	930772	1165171	62.69%	7.254%
16	10.792	1475	1479	1492	rVB4	11717	22986	1.24%	0.143%
17	11.398	1567	1582	1585	rBV	501902	818824	44.06%	5.098%
18	11.469	1590	1594	1598	rVB	64464	85028	4.58%	0.529%
19	11.621	1615	1620	1628	rVB	31169	44193	2.38%	0.275%
20	11.774	1641	1646	1650	rBV3	14957	19145	1.03%	0.119%
21	11.916	1662	1670	1682	rBV3	157144	287983	15.50%	1.793%
22	12.010	1682	1686	1692	rVB2	36040	57324	3.08%	0.357%
23	12.604	1782	1787	1794	rBV	219812	278005	14.96%	1.731%
24	12.704	1799	1804	1810	rBV	34625	56029	3.01%	0.349%
25	12.833	1819	1826	1831	rBV	142484	214976	11.57%	1.338%
26	12.980	1841	1851	1856	rBV	1081940	1393737	74.99%	8.677%
27	13.051	1856	1863	1874	rVB3	66021	166612	8.96%	1.037%
28	13.163	1874	1882	1886	rBV	27448	43417	2.34%	0.270%
29	13.227	1889	1893	1896	rBV	20338	21546	1.16%	0.134%
30	13.898	1999	2007	2019	rVB4	81246	234194	12.60%	1.458%
31	14.027	2021	2029	2041	rVB2	319690	544445	29.30%	3.390%
32	14.527	2104	2114	2123	rBV	99836	204079	10.98%	1.271%
33	15.068	2201	2206	2212	rBV	61276	139868	7.53%	0.871%
34	15.127	2212	2216	2222	rVV	59172	119820	6.45%	0.746%
35	15.374	2253	2258	2263	rBV	28423	45193	2.43%	0.281%
36	15.433	2263	2268	2274	rVB	46019	68605	3.69%	0.427%

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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

37	15.498	2274	2279	2293	rBV	231064	384319	20.68%	2.393%
38	15.804	2324	2331	2338	rBV	41047	92292	4.97%	0.575%
39	16.162	2385	2392	2409	rBV10	18243	62047	3.34%	0.386%
40	16.586	2456	2464	2473	rVB	26641	68704	3.70%	0.428%
41	16.909	2514	2519	2523	rBV5	11396	23643	1.27%	0.147%
42	16.962	2524	2528	2535	rVB2	17007	34479	1.86%	0.215%
43	17.480	2610	2616	2626	rVB4	13747	43302	2.33%	0.270%

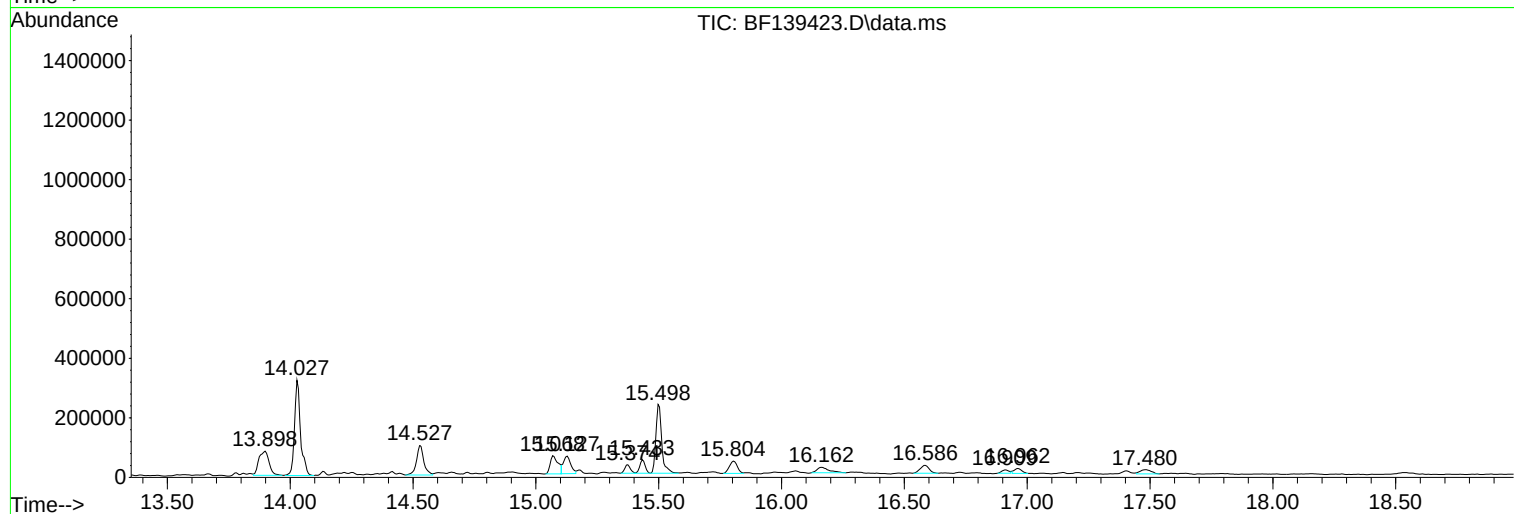
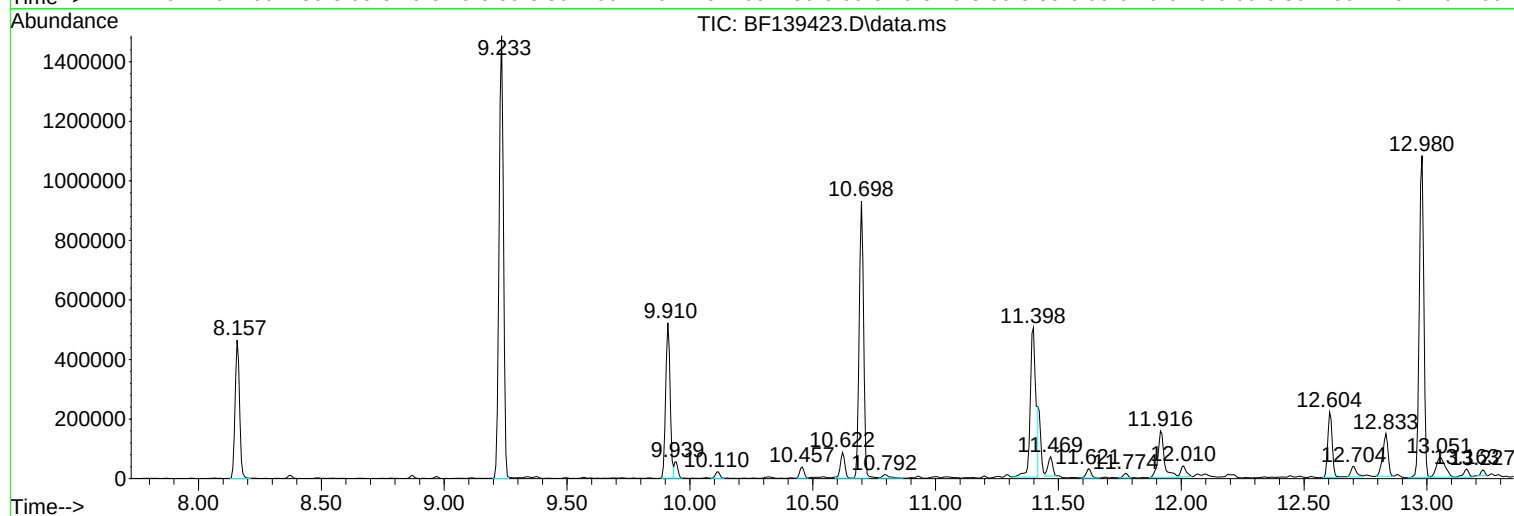
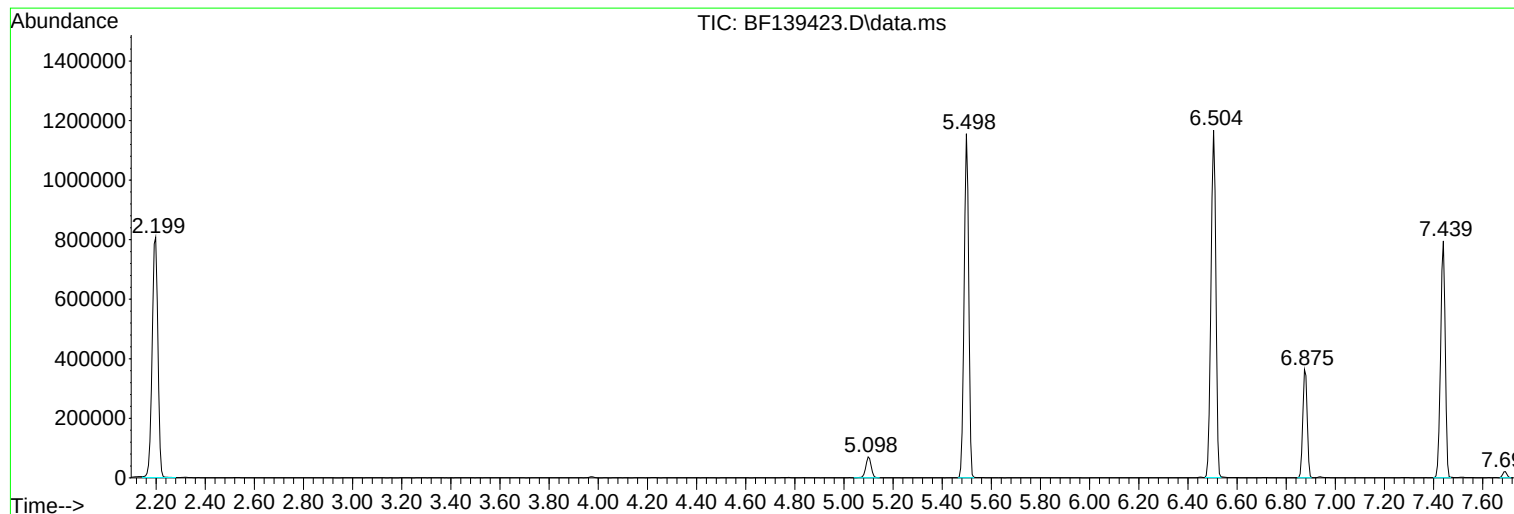
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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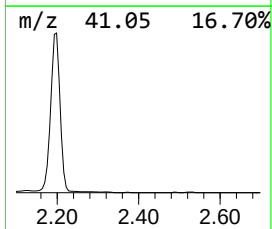
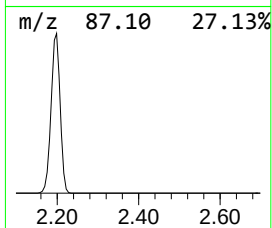
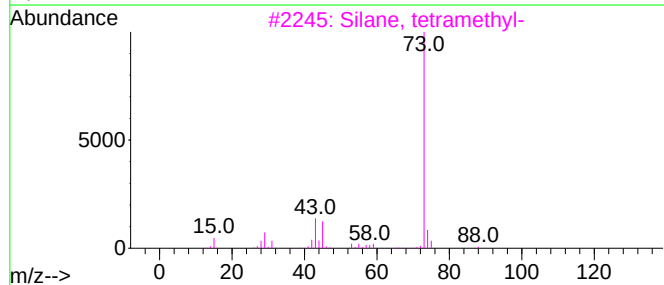
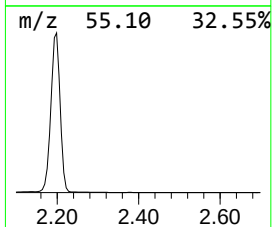
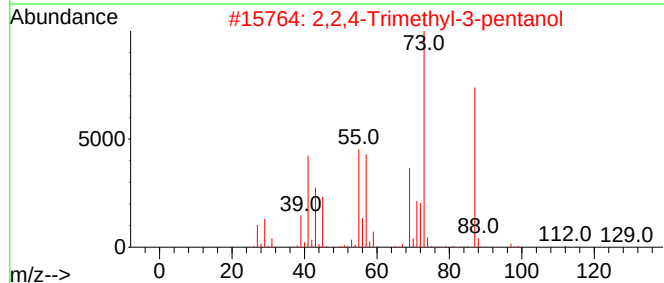
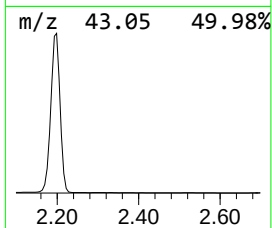
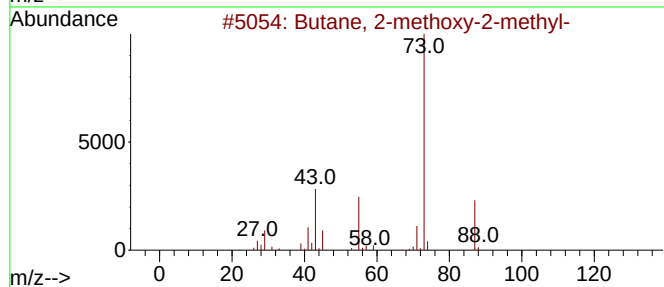
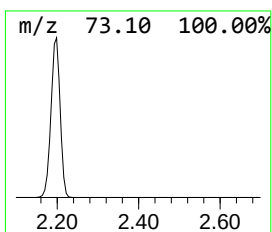
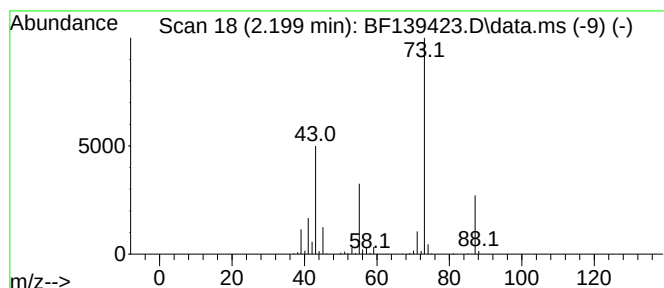
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	56.99 ng	1286700	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Misc :
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Instrument :
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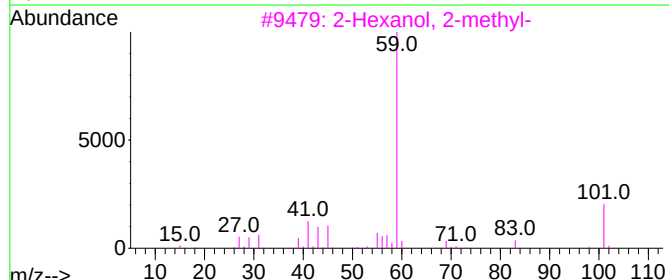
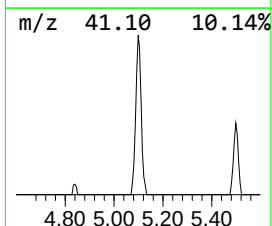
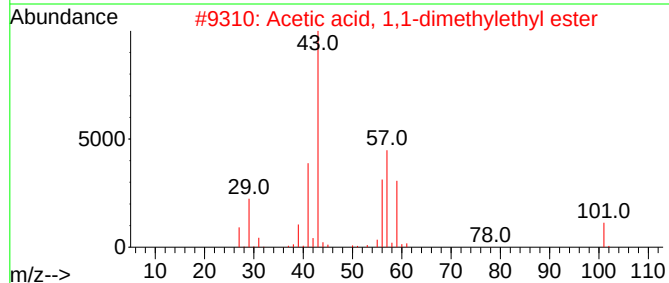
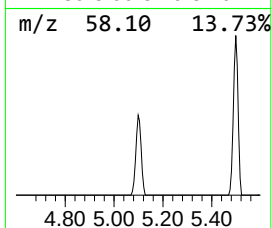
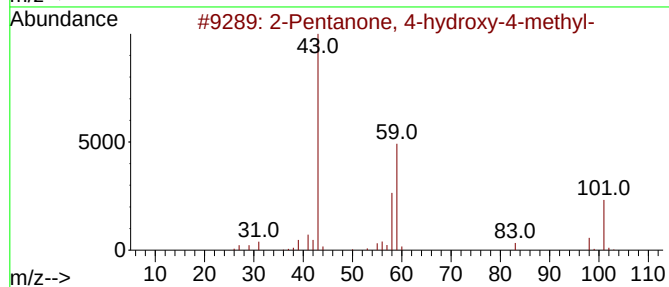
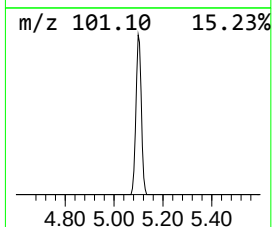
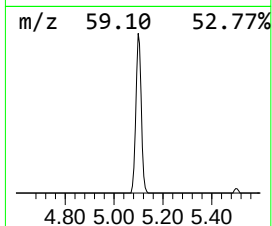
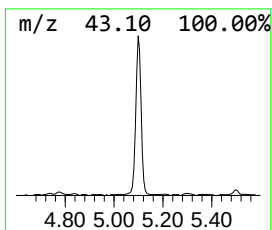
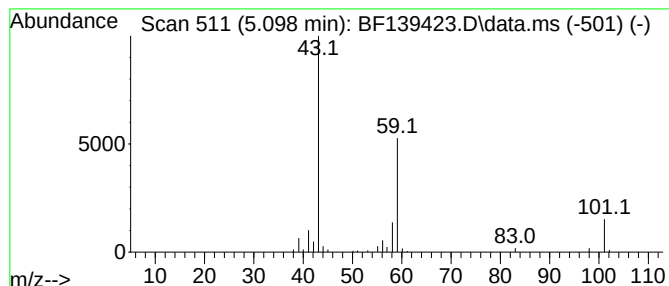
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	4.75 ng	107281	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	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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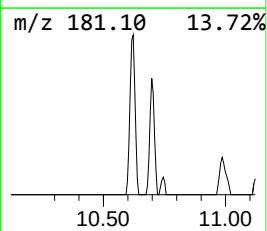
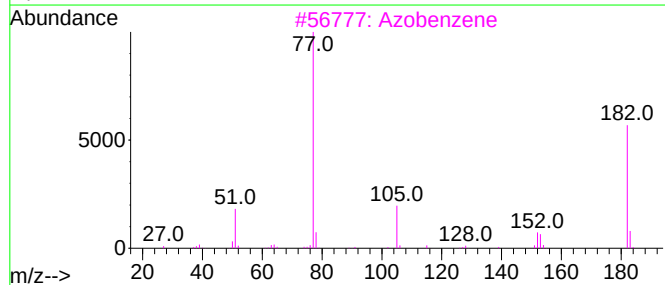
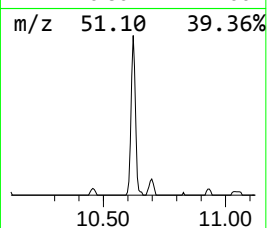
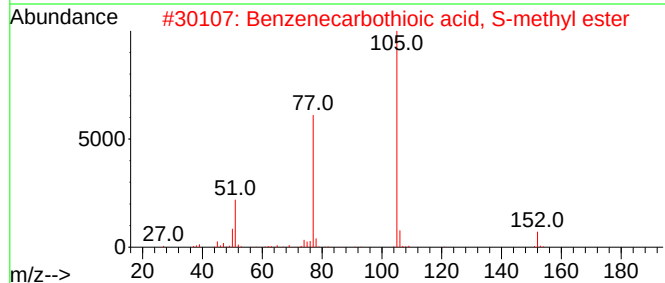
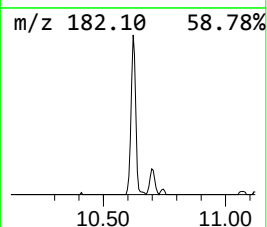
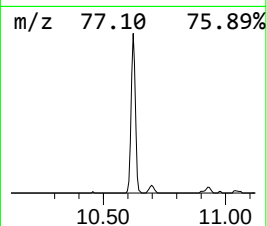
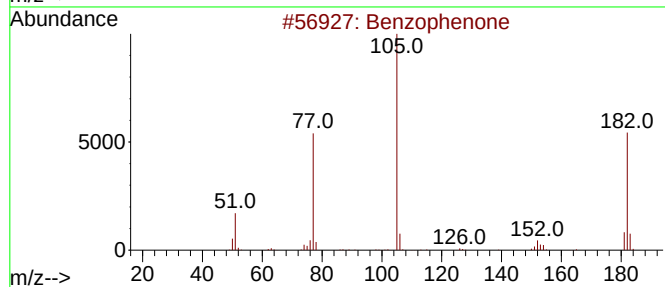
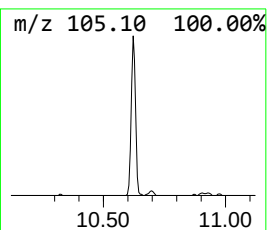
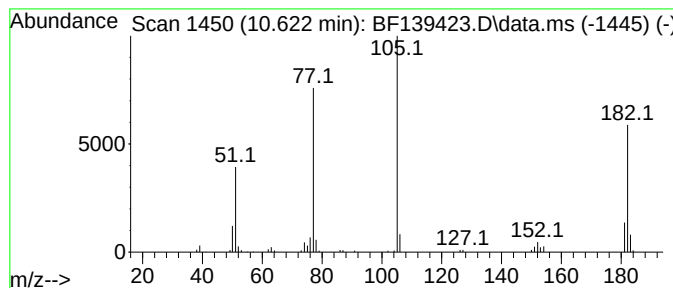
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	3.35 ng	108818	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	76
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			Benzoylformic acid	150	C8H6O3	000611-73-4	58
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53



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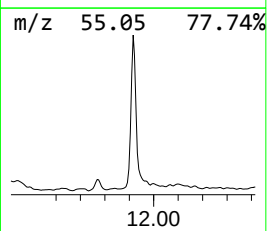
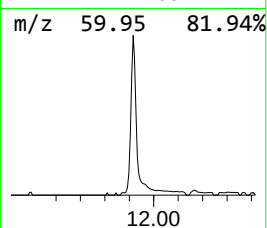
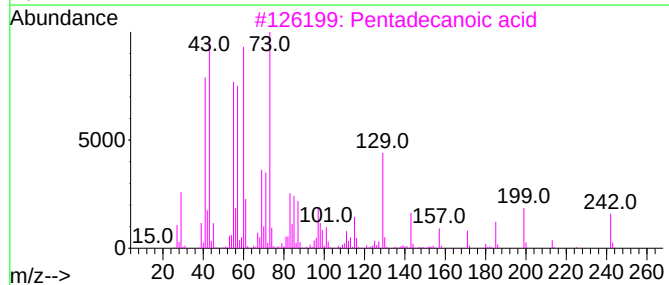
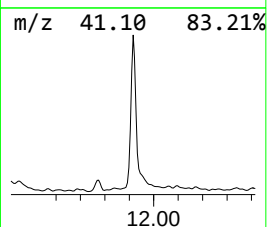
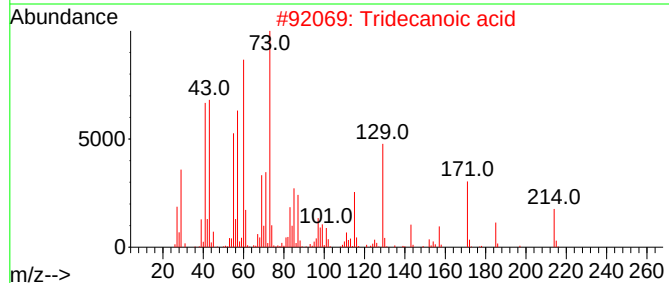
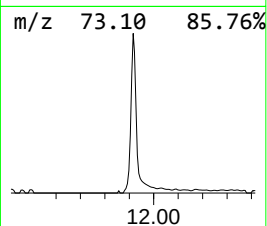
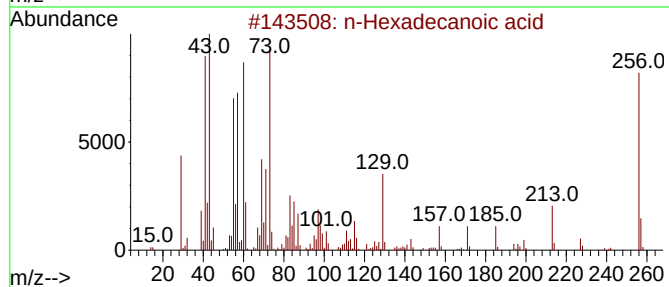
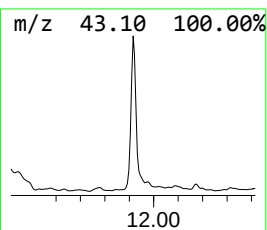
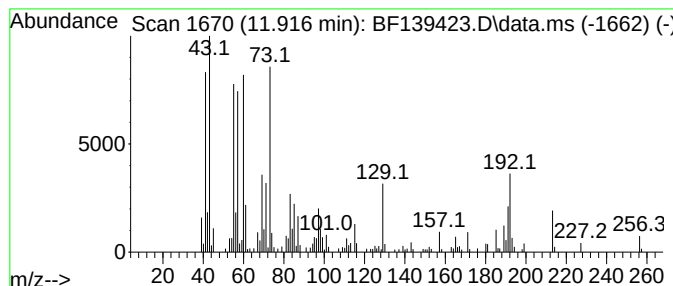
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.03 ng	287983	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Undecanoic acid	186	C11H22O2	000112-37-8	49
5			n-Decanoic acid	172	C10H20O2	000334-48-5	45



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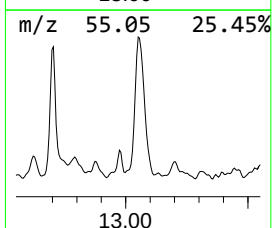
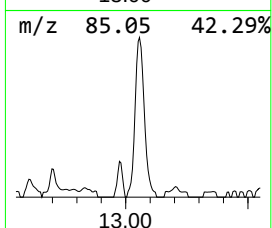
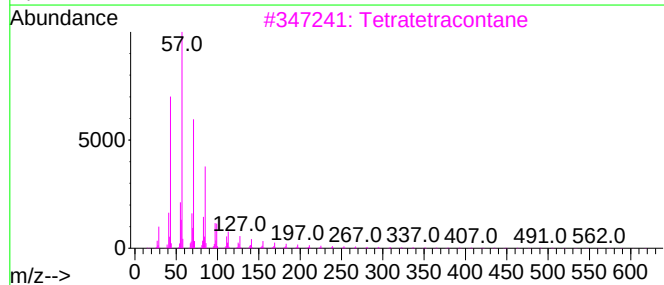
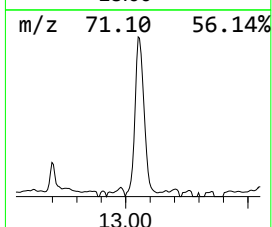
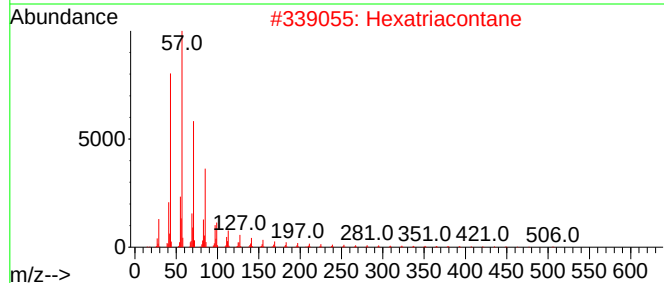
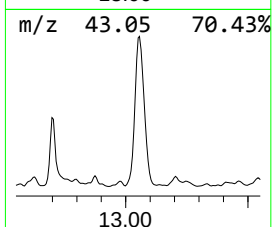
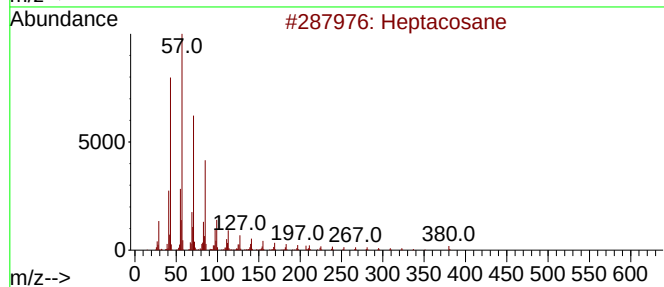
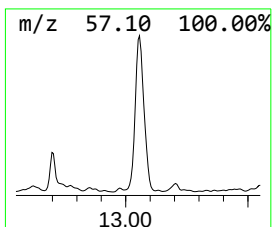
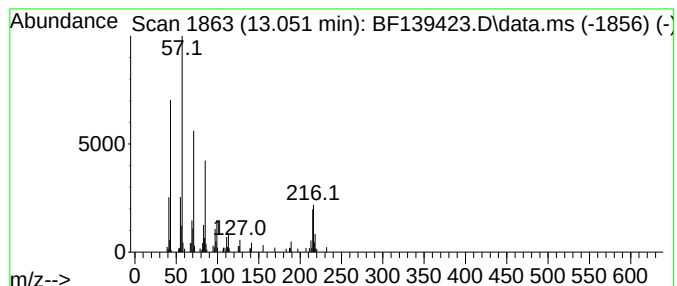
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	6.12 ng	166612	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	70
2			Hexatriacontane	507	C36H74	000630-06-8	70
3			Tetratetracontane	619	C44H90	007098-22-8	70
4			Hentriacontane	437	C31H64	000630-04-6	70
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2-TANK17

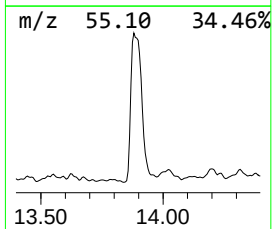
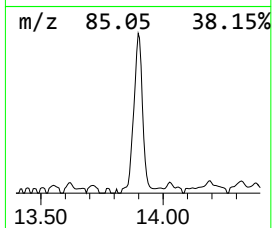
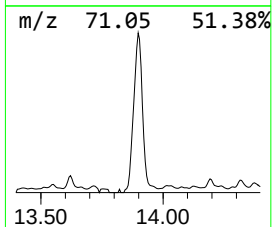
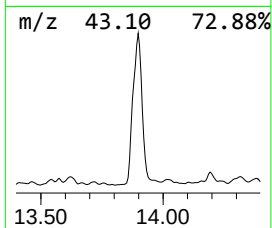
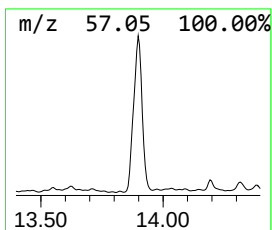
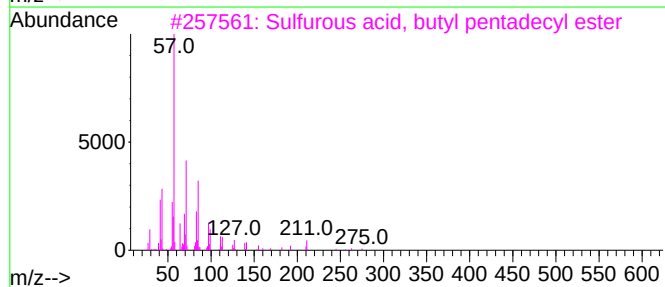
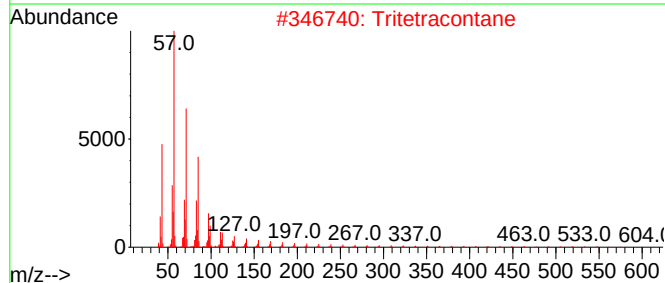
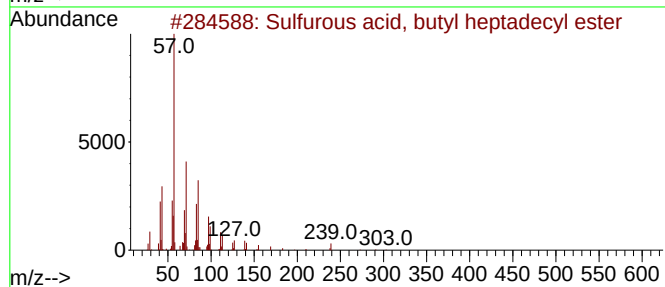
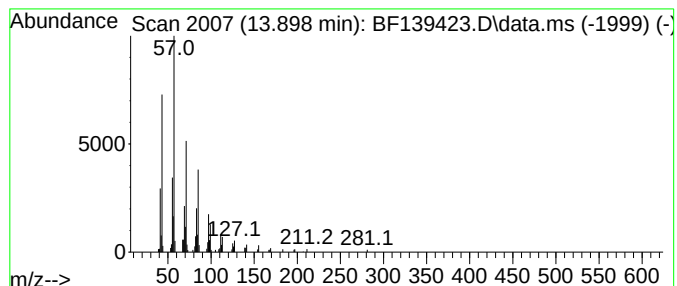
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Sulfurous acid, butyl hepta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	8.60 ng	234194	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2			Tritetracontane	605	C43H88	007098-21-7	91
3			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	91
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
5			Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
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Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

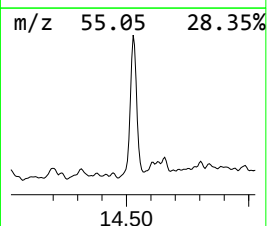
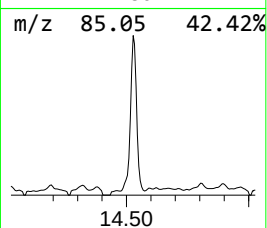
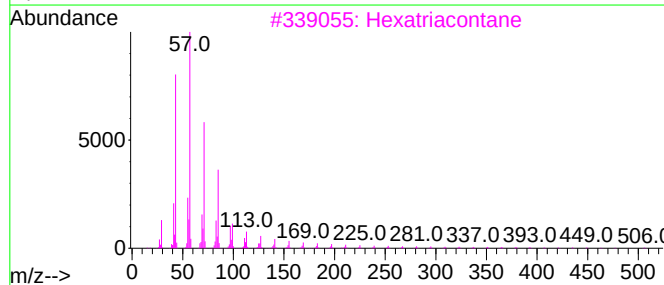
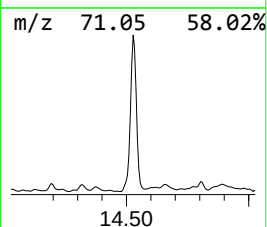
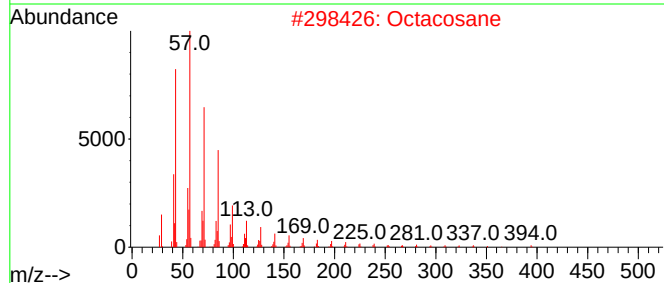
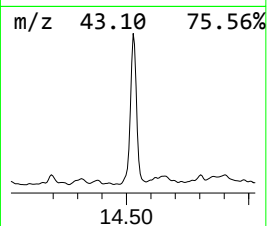
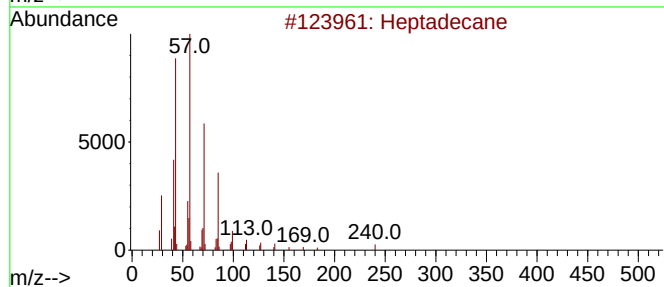
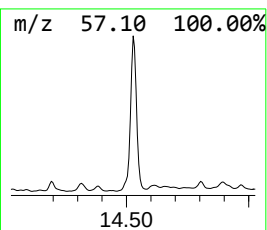
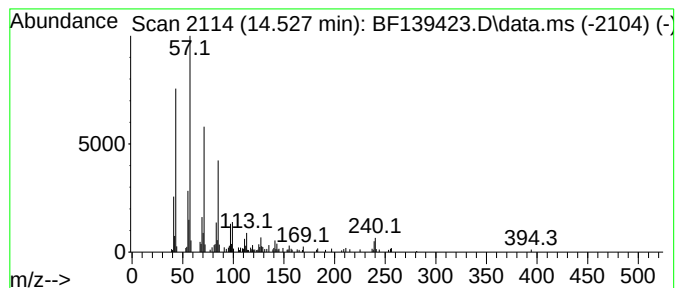
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.527	7.50 ng	204079	Chrysene-d12	14.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Octacosane	394	C28H58	000630-02-4	93
3	Hexatriacontane	507	C36H74	000630-06-8	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-2-TANK17

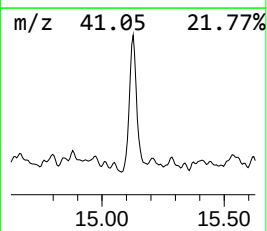
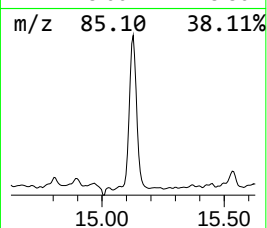
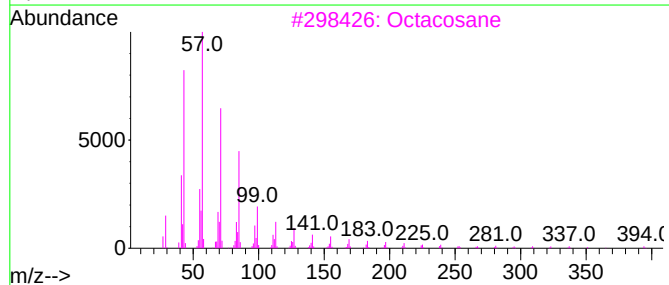
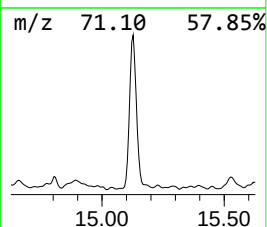
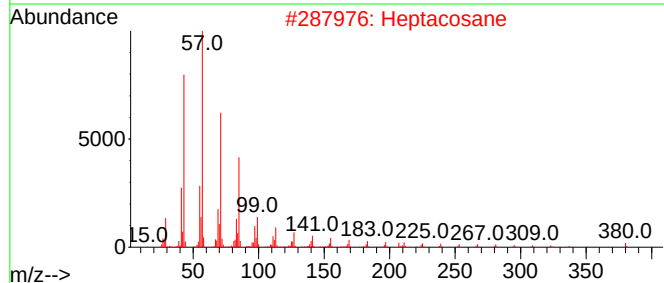
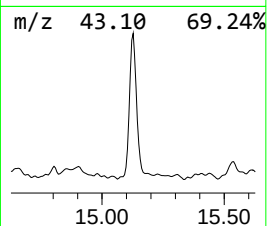
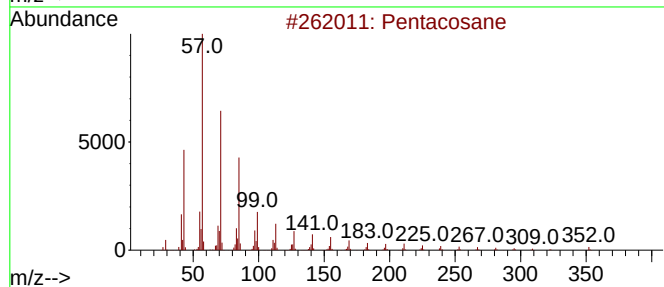
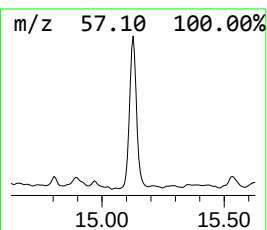
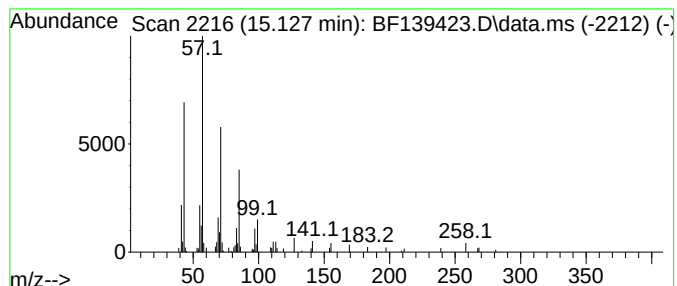
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	6.24 ng	119820	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Nonadecane	268	C19H40	000629-92-5	90
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-2-TANK17

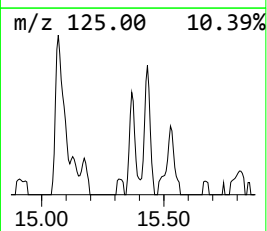
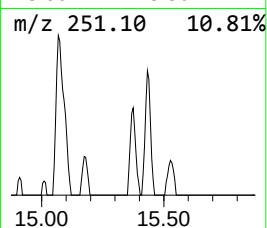
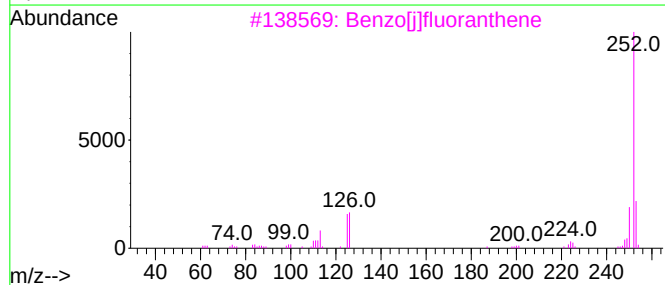
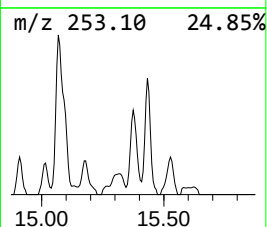
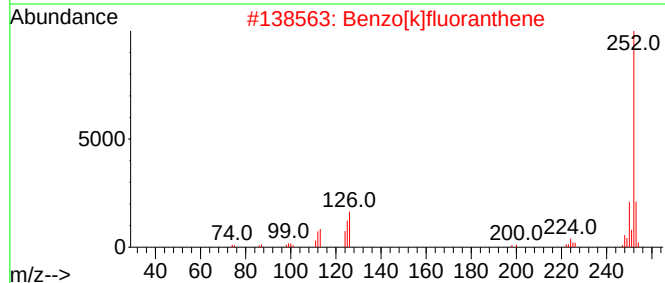
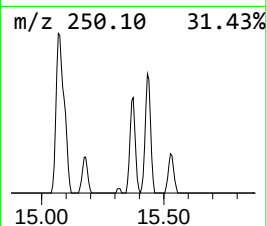
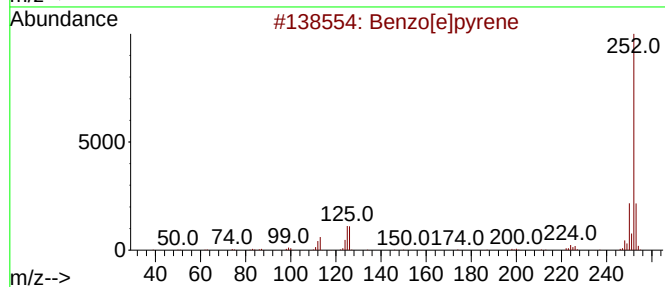
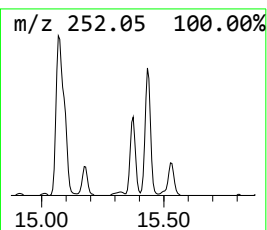
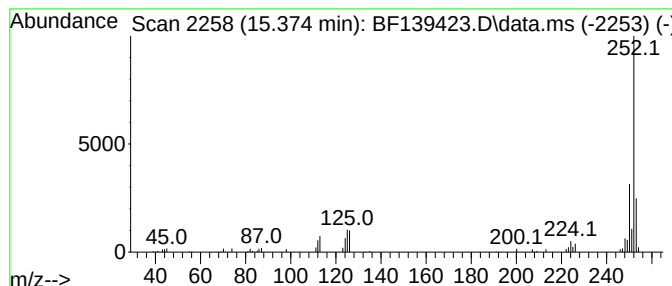
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	2.35 ng	45193	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
SW-2-TANK17

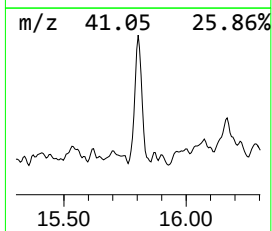
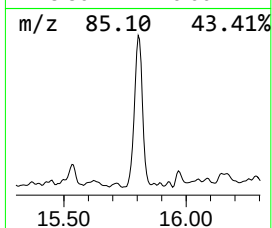
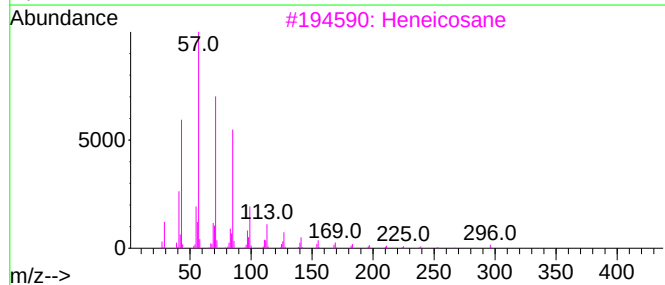
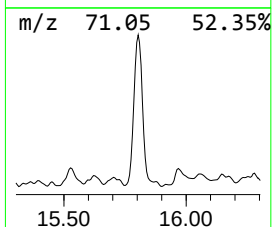
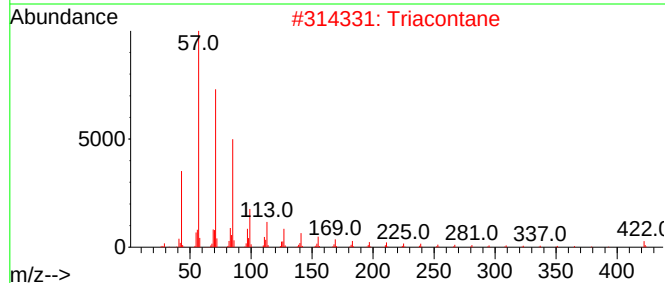
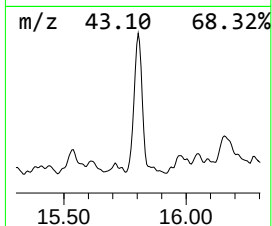
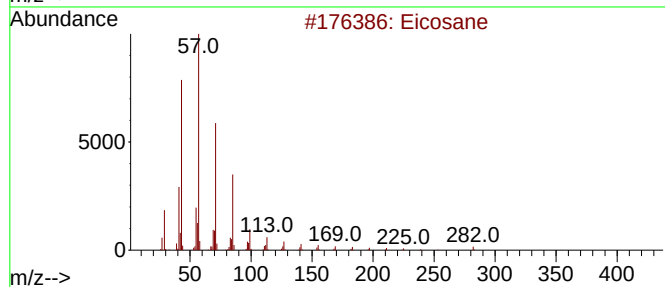
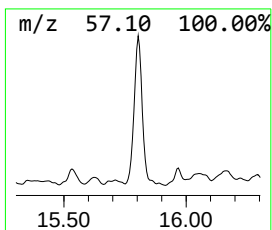
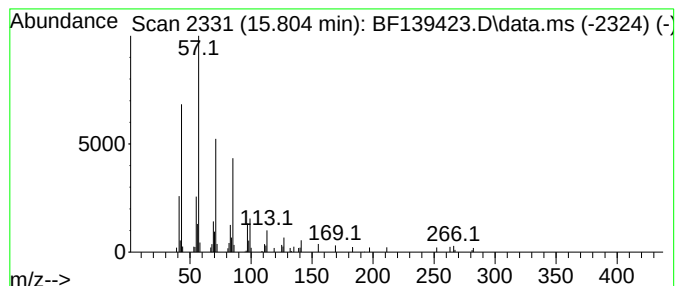
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.804	4.80 ng	92292	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Triacontane	422	C30H62	000638-68-6	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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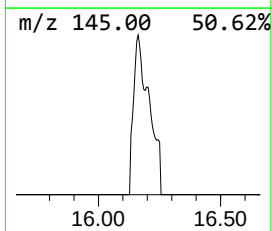
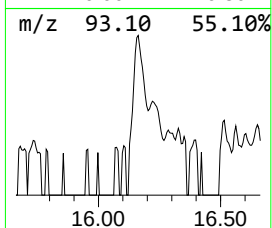
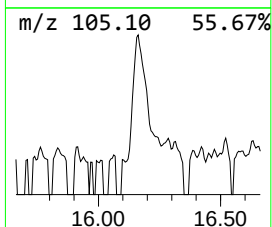
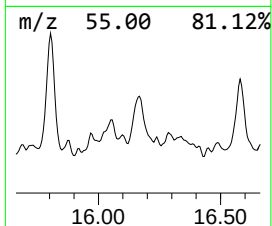
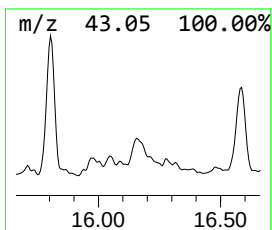
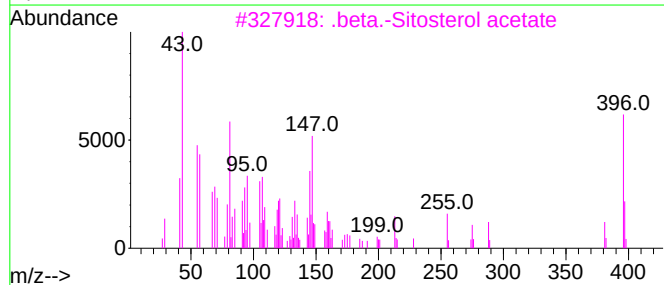
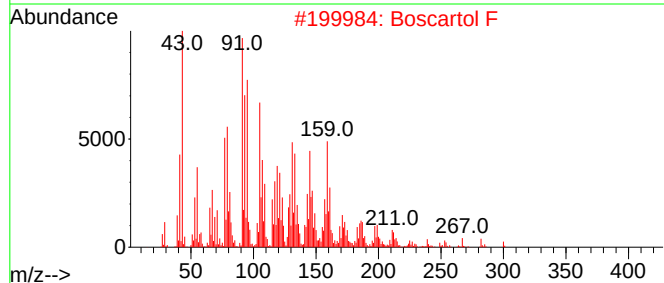
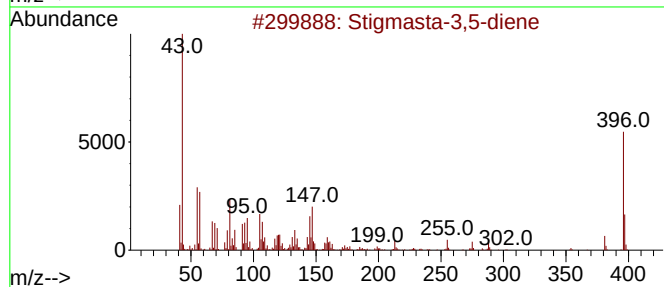
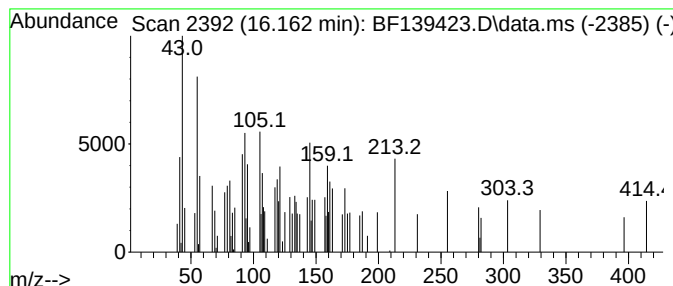
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown16.162 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.162	3.23 ng	62047	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Stigmasta-3,5-diene	396	C29H48	004970-37-0	27
2		Boscartol F	300	C20H28O2	1486443-17-7	16
3		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	12
4		Ledene oxide-(II)	220	C15H24O	1000159-36-7	12
5		Z,Z-10,12-Hexadecadien-1-ol acetate	280	C18H32O2	1000130-89-5	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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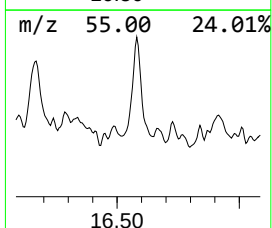
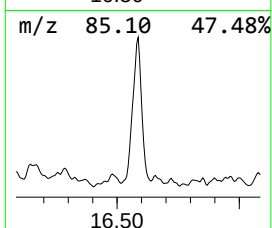
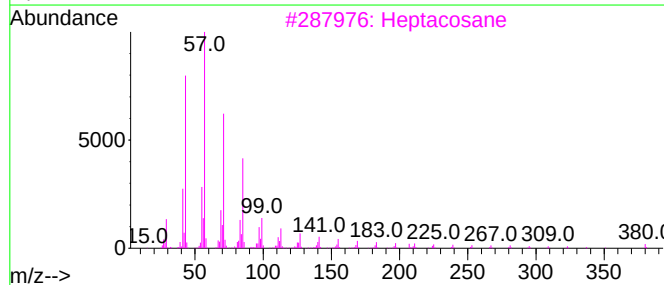
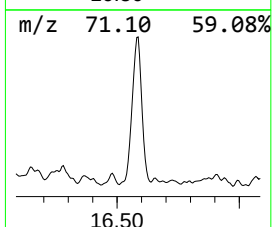
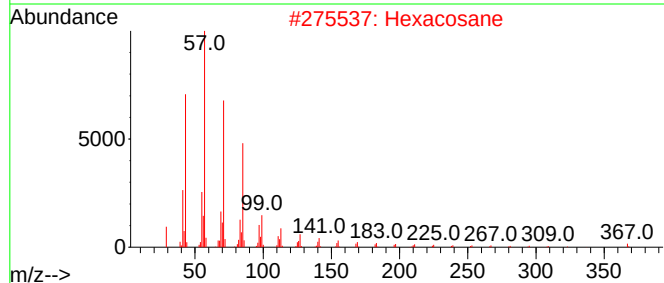
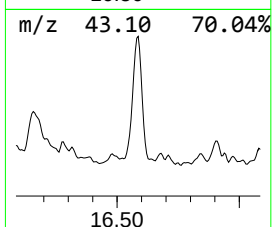
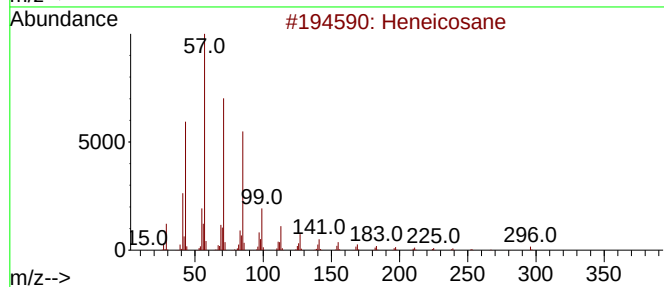
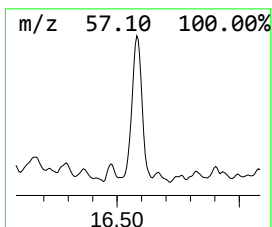
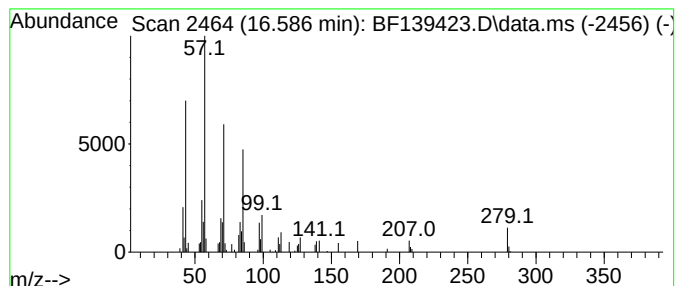
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	3.58 ng	68704	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heptacosane	380	C27H56	000593-49-7	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Hexatriacontane	507	C36H74	000630-06-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2-TANK17

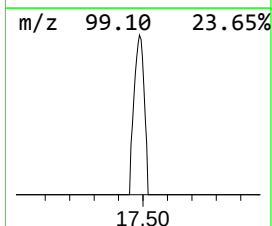
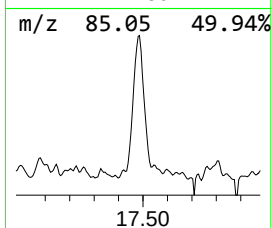
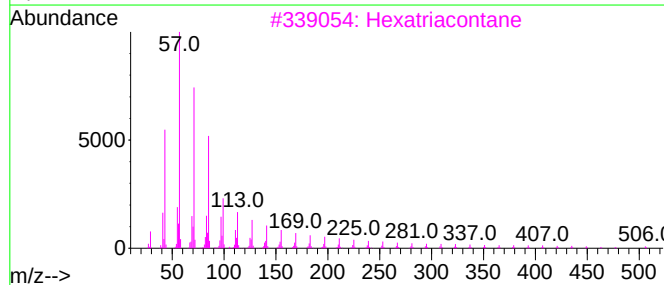
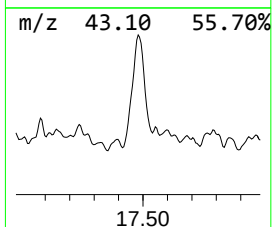
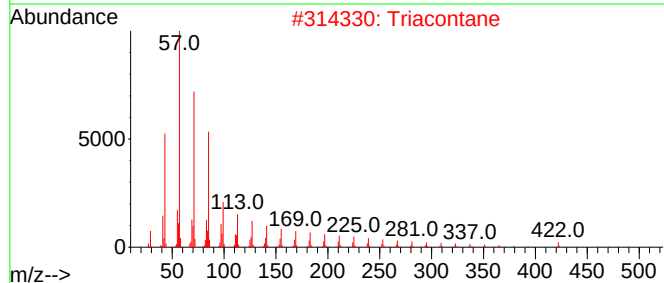
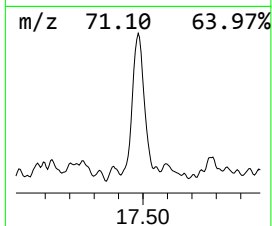
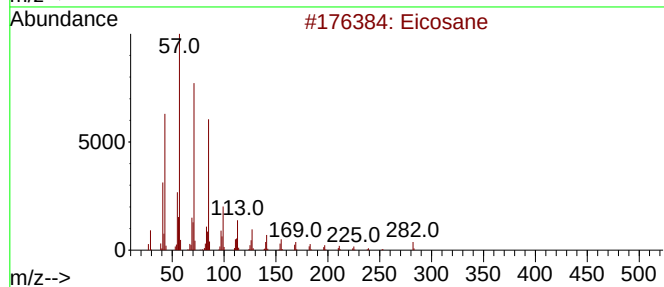
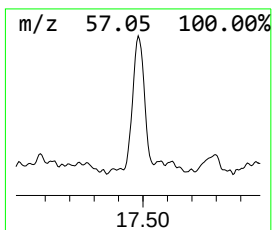
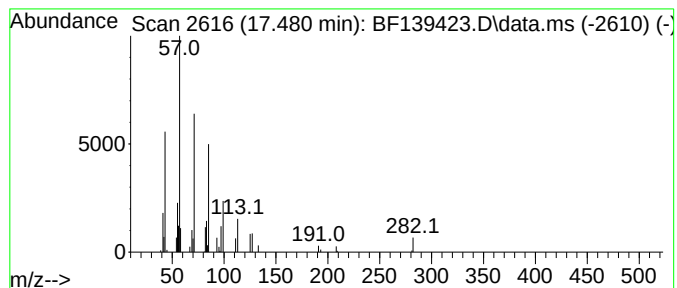
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Triacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	2.25 ng	43302	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	91
2		Triacontane	422	C30H62	000638-68-6	78
3		Hexatriacontane	507	C36H74	000630-06-8	78
4		Nonacosane	408	C29H60	000630-03-5	78
5		Tetratriacontane	479	C34H70	014167-59-0	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139423.D
Acq On : 18 Sep 2024 13:21
Operator : RC/JU
Sample : P4015-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2-TANK17

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.199	57.0	ng	1286700	1	6.875	451574	20.0
2-Pentanone, 4-...	5.098	4.8	ng	107281	1	6.875	451574	20.0
Benzophenone	10.621	3.4	ng	108818	3	9.910	649930	20.0
n-Hexadecanoic ...	11.916	7.0	ng	287983	4	11.398	818824	20.0
Heptacosane	13.051	6.1	ng	166612	5	14.027	544445	20.0
Sulfurous acid,...	13.898	8.6	ng	234194	5	14.027	544445	20.0
Heptadecane	14.527	7.5	ng	204079	5	14.027	544445	20.0
Pentacosane	15.127	6.2	ng	119820	6	15.498	384319	20.0
Benzo[e]pyrene	15.374	2.4	ng	45193	6	15.498	384319	20.0
Eicosane	15.804	4.8	ng	92292	6	15.498	384319	20.0
unknown16.162	16.162	3.2	ng	62047	6	15.498	384319	20.0
Heneicosane	16.586	3.6	ng	68704	6	15.498	384319	20.0
Triacontane	17.480	2.3	ng	43302	6	15.498	384319	20.0