

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
 Data File : BF140515.D
 Acq On : 20 Nov 2024 22:13
 Operator : RC/JU
 Sample : P4822-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SOIL-6

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140515.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	21	rVB	892084	1466273	62.34%	6.821%
2	5.098	506	511	521	rVB	37924	57936	2.46%	0.269%
3	5.304	538	546	553	rBV	16511	27850	1.18%	0.130%
4	5.504	574	580	597	rBV	1618613	2173719	92.42%	10.111%
5	6.510	745	751	769	rBV	1581978	2123716	90.29%	9.879%
6	6.875	808	813	818	rBV	510267	627102	26.66%	2.917%
7	7.434	902	908	917	rBV	1057474	1360425	57.84%	6.328%
8	7.686	945	951	962	rBV	26617	42063	1.79%	0.196%
9	8.151	1025	1030	1043	rBV	544126	724501	30.80%	3.370%
10	9.228	1207	1213	1223	rBV	1812456	2340791	99.52%	10.888%
11	9.910	1323	1329	1341	rVB	527303	701959	29.84%	3.265%
12	10.622	1444	1450	1456	rBV	374853	478134	20.33%	2.224%
13	10.698	1458	1463	1473	rVV	924495	1205652	51.26%	5.608%
14	10.927	1498	1502	1511	rVB	63237	85012	3.61%	0.395%
15	11.063	1521	1525	1534	rBV6	21131	34499	1.47%	0.160%
16	11.398	1576	1582	1592	rBV	544663	812921	34.56%	3.781%
17	11.627	1614	1621	1627	rBV2	14544	39694	1.69%	0.185%
18	11.921	1663	1671	1683	rVV2	316701	571498	24.30%	2.658%
19	12.016	1683	1687	1695	rVB3	24119	55348	2.35%	0.257%
20	12.086	1695	1699	1705	rBV4	22472	43772	1.86%	0.204%
21	12.416	1751	1755	1759	rBV	21176	33507	1.42%	0.156%
22	12.616	1781	1789	1800	rBV	199818	484270	20.59%	2.253%
23	12.710	1801	1805	1816	rVB3	70261	139840	5.95%	0.650%
24	12.845	1822	1828	1835	rVB	113812	168358	7.16%	0.783%
25	12.980	1846	1851	1859	rBV	1738235	2352048	100.00%	10.941%
26	13.204	1886	1889	1893	rBV	35937	45902	1.95%	0.214%
27	13.886	2000	2005	2022	rBV3	103927	238982	10.16%	1.112%
28	14.045	2024	2032	2040	rBV2	539673	865001	36.78%	4.024%
29	14.515	2108	2112	2114	rBV	62084	89468	3.80%	0.416%
30	14.898	2174	2177	2184	rVB	82988	112482	4.78%	0.523%
31	15.168	2218	2223	2228	rVB	214146	304191	12.93%	1.415%
32	15.545	2282	2287	2298	rVB	317671	549810	23.38%	2.557%
33	15.998	2359	2364	2370	rVB	165134	275960	11.73%	1.284%
34	18.209	2734	2740	2751	rVB3	179952	465006	19.77%	2.163%
35	18.686	2815	2821	2838	rVB2	132443	400307	17.02%	1.862%

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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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

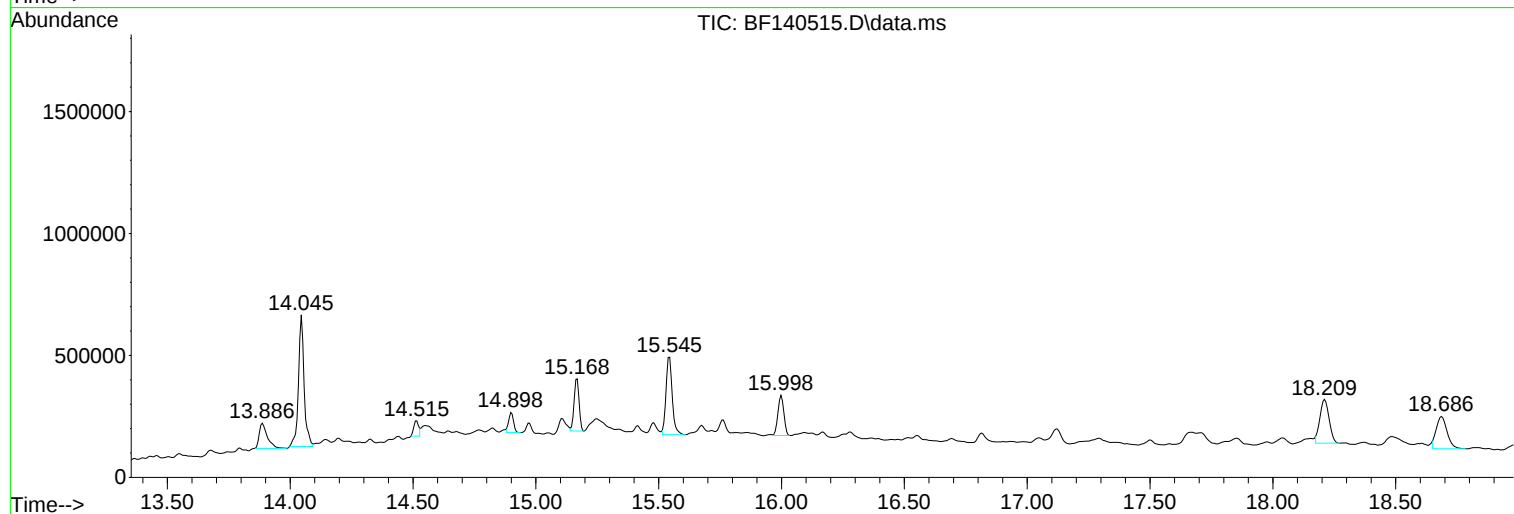
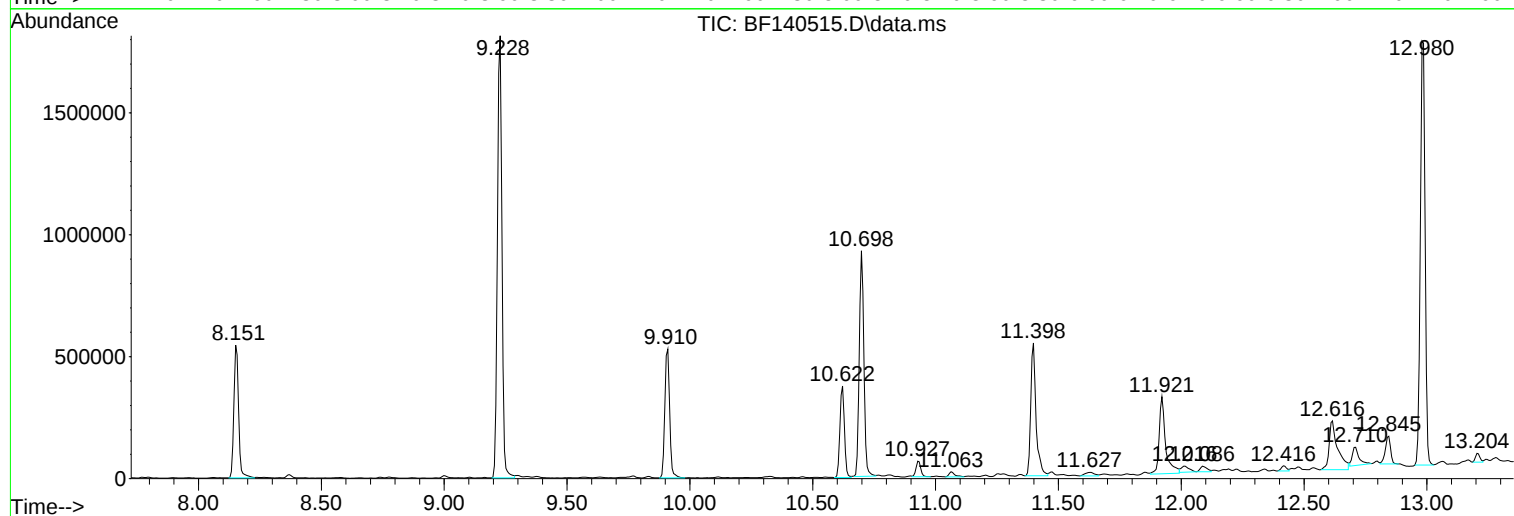
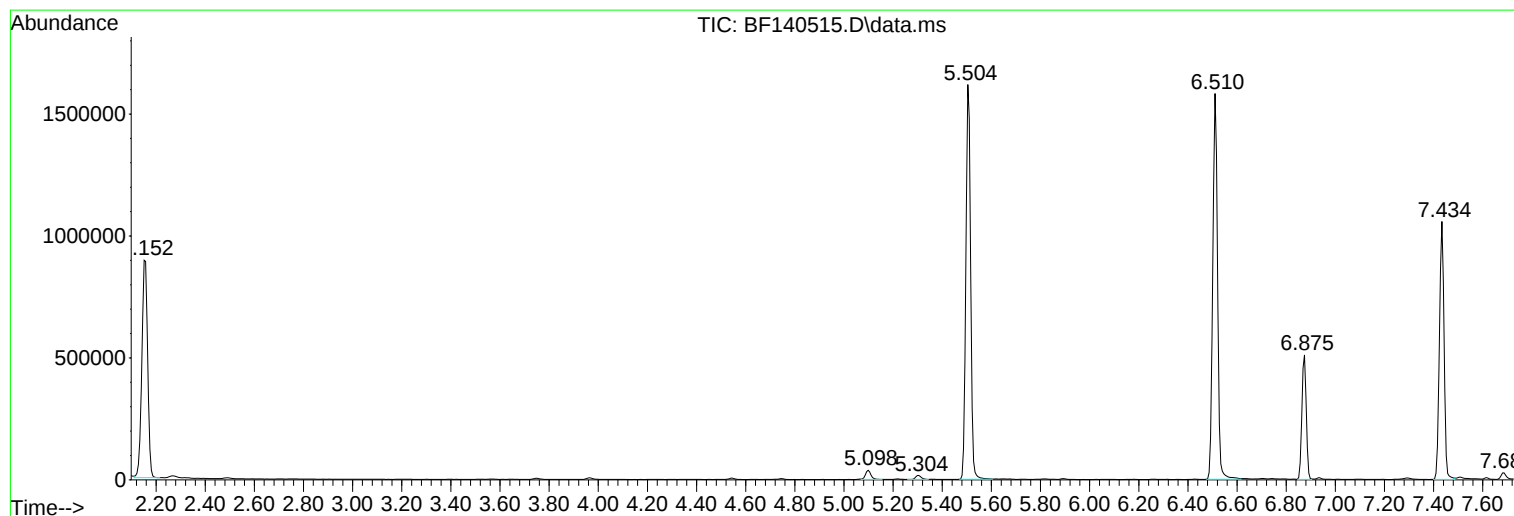
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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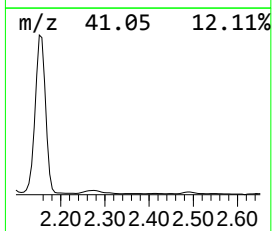
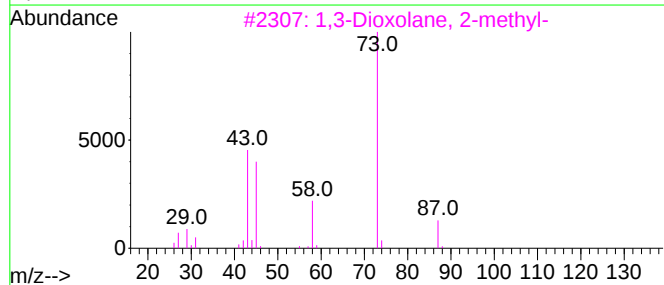
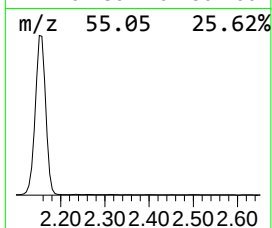
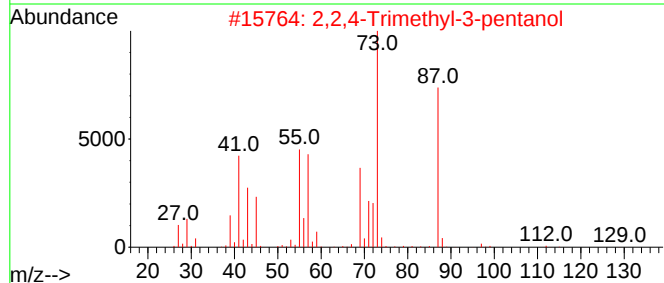
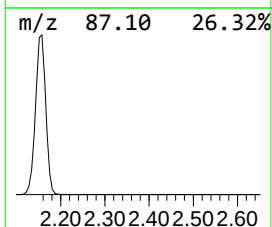
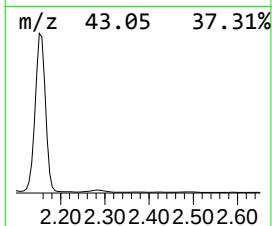
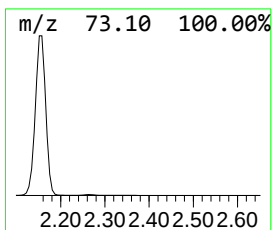
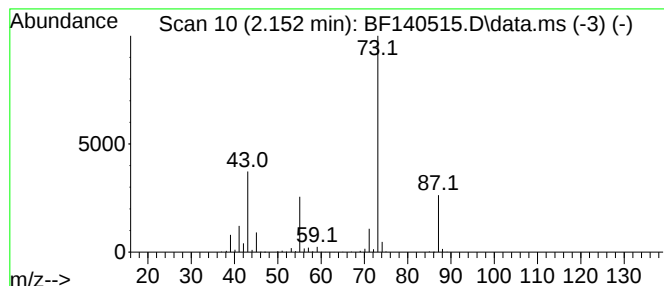
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	46.76 ng	1466270	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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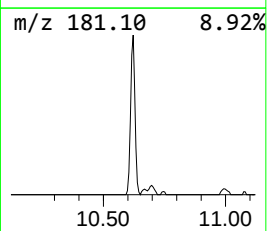
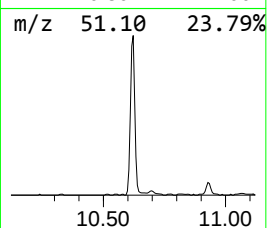
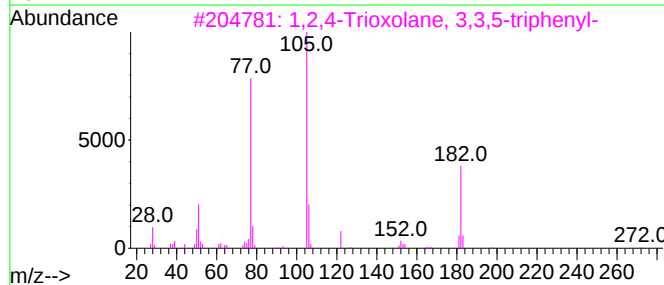
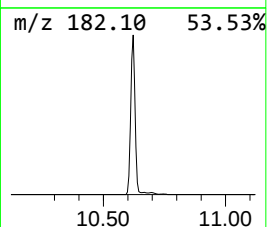
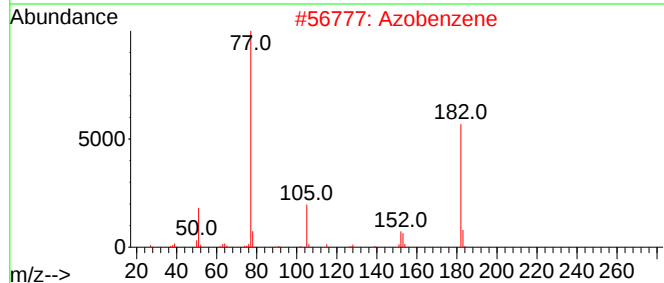
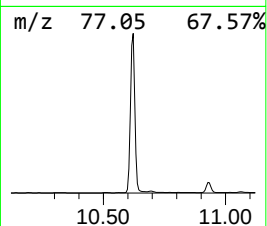
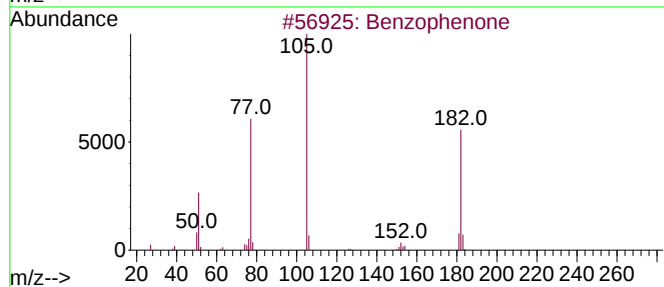
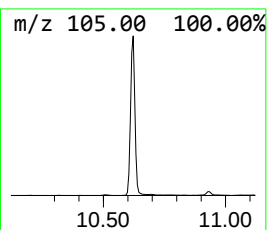
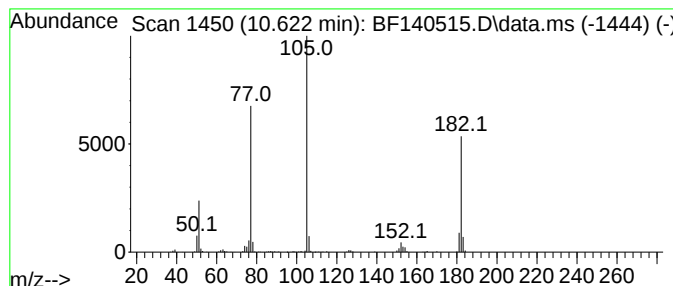
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	13.62 ng	478134	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Azobenzene	182	C12H10N2	000103-33-3	72
3		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
4		N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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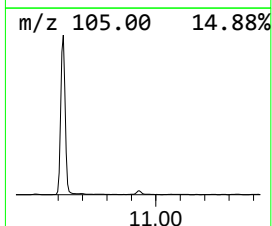
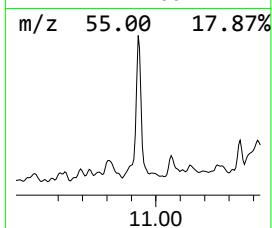
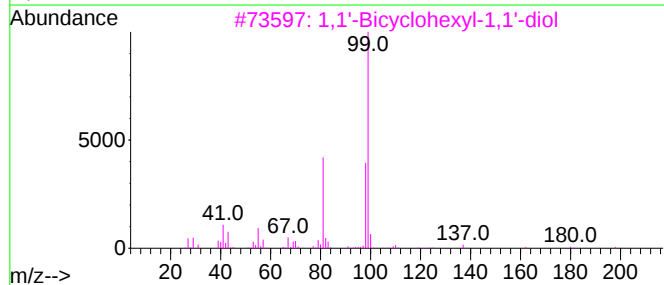
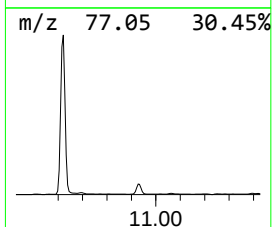
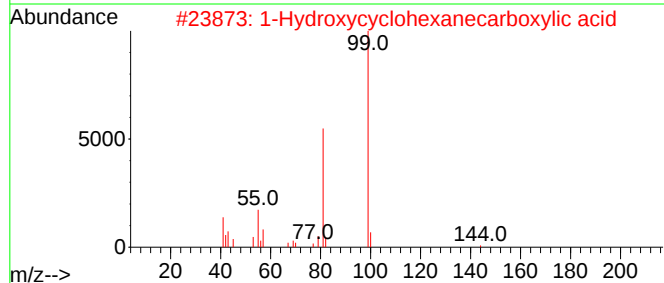
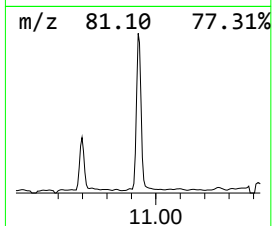
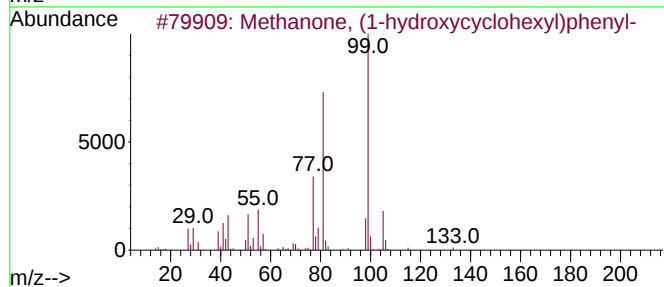
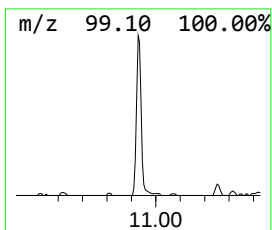
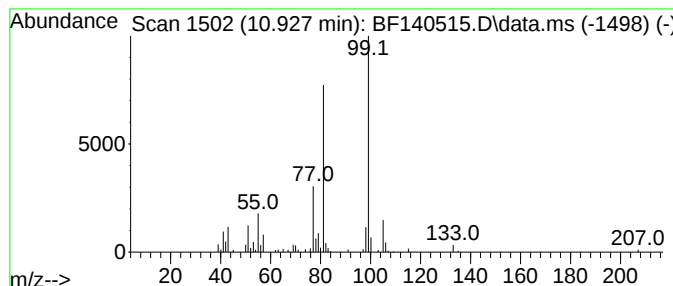
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.927	2.09 ng	85012	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3			1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	36
4			Isothiazole, 3-methyl-	99	C4H5NS	000693-92-5	16
5			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	12



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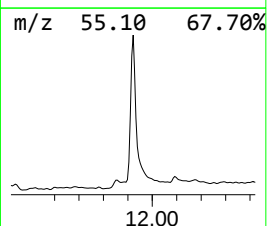
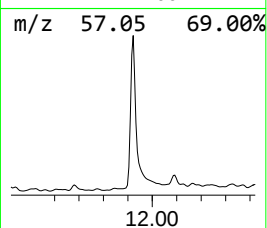
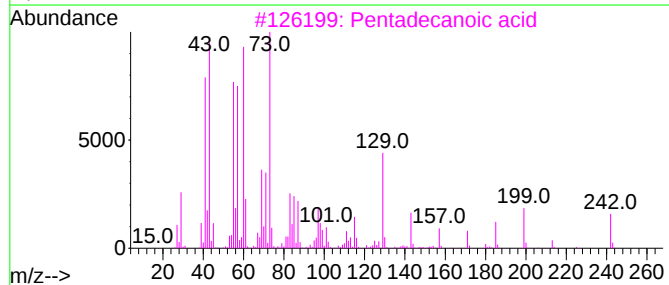
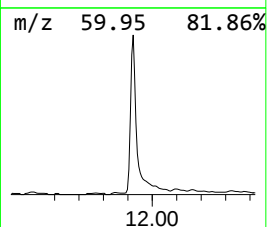
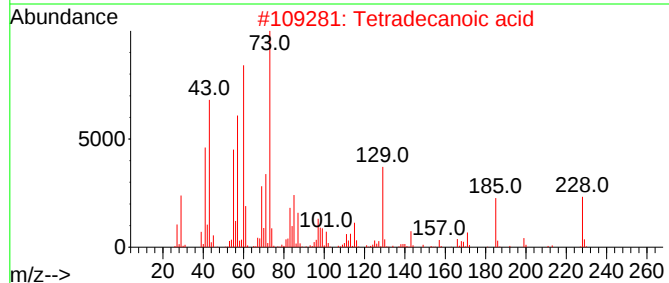
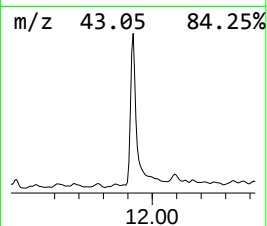
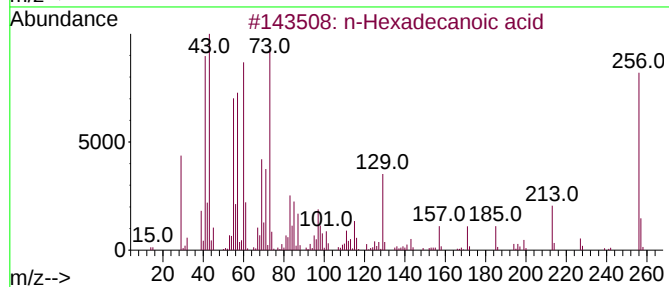
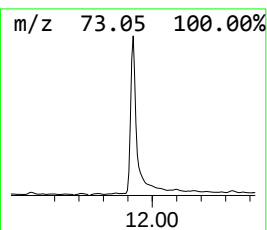
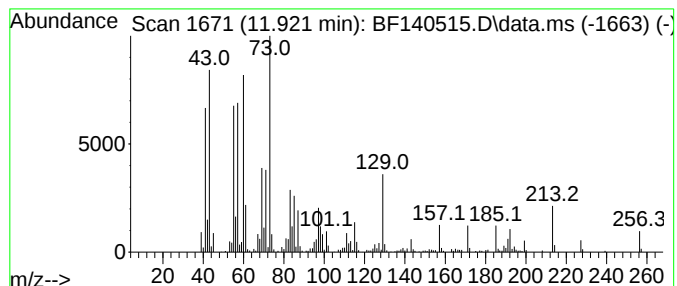
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	14.06 ng	571498	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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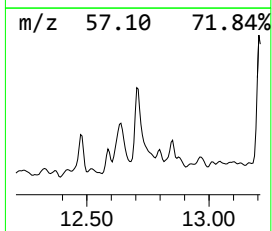
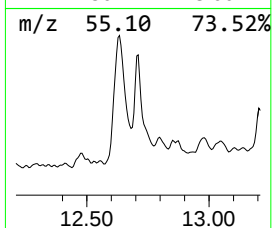
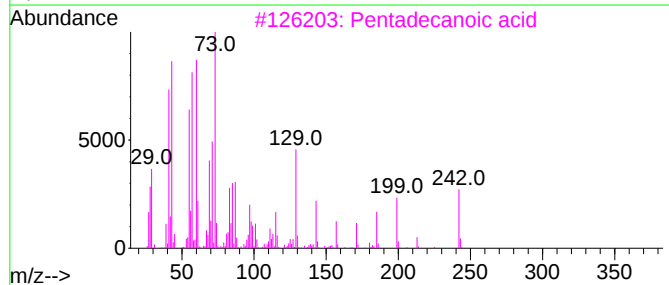
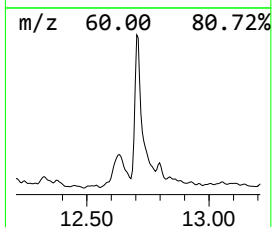
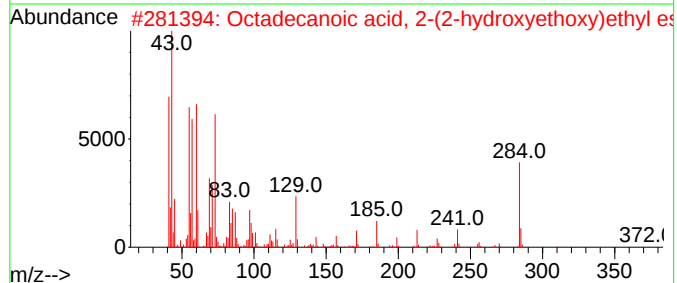
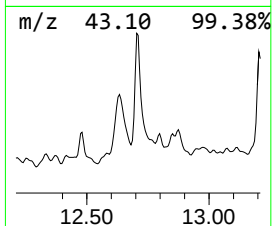
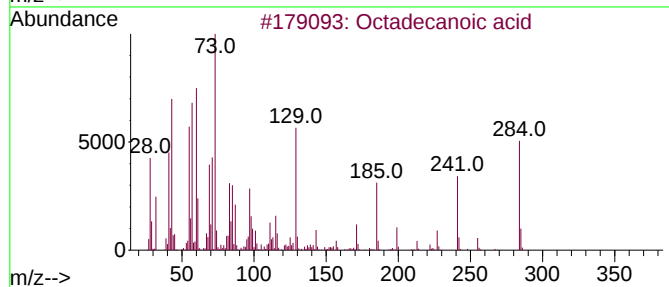
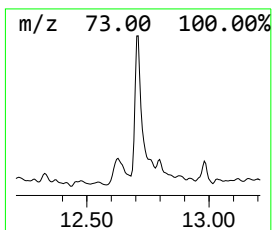
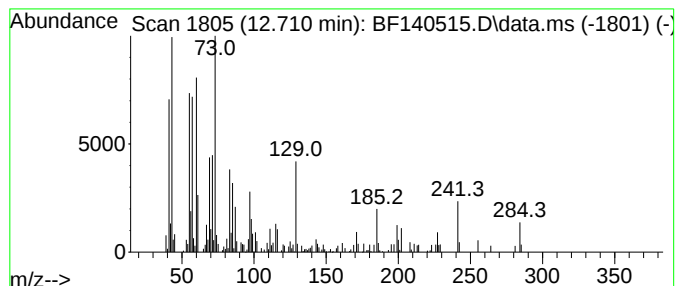
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Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	3.44 ng	139840	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
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Acq On : 20 Nov 2024 22:13
Operator : RC/JU
Sample : P4822-12
Misc :
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Instrument :
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ClientSampleId :
SOIL-6

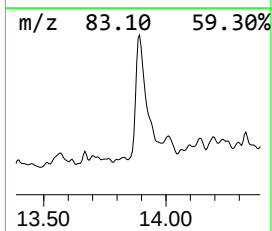
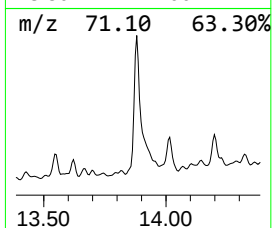
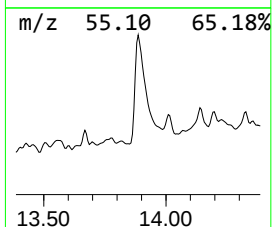
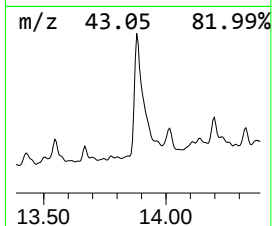
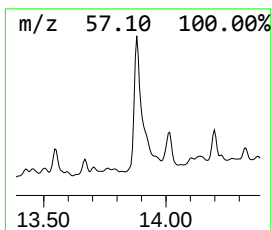
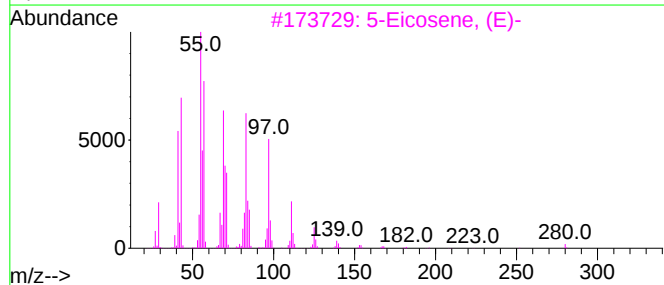
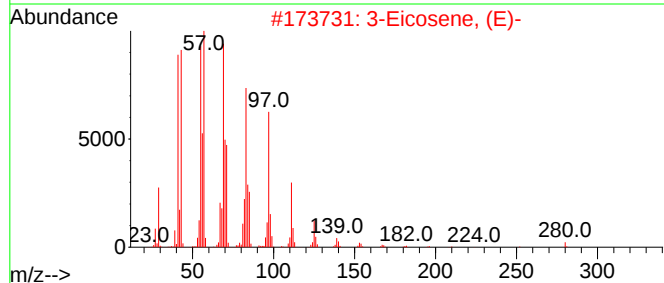
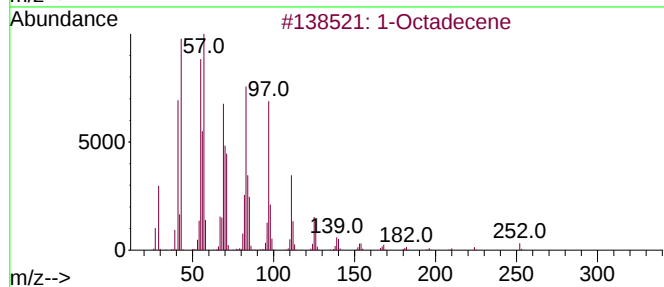
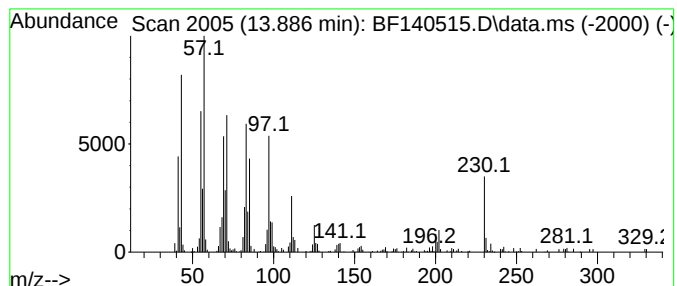
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.53 ng	238982	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	95
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	94
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	89
5			Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
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Sample : P4822-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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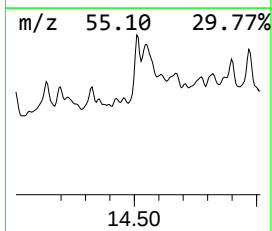
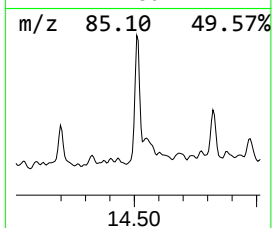
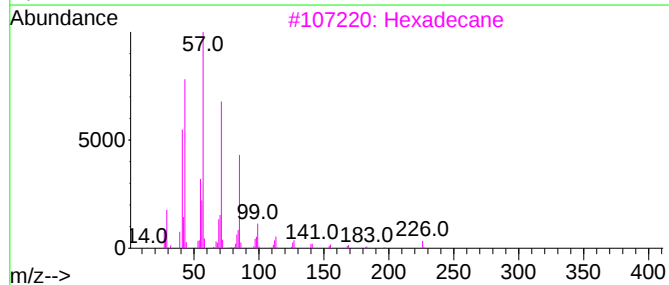
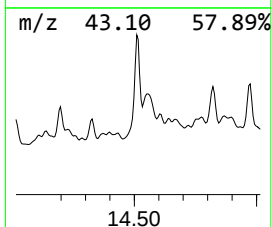
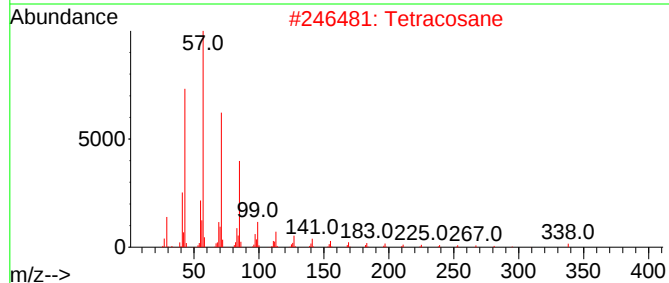
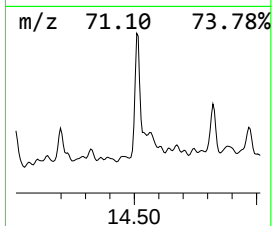
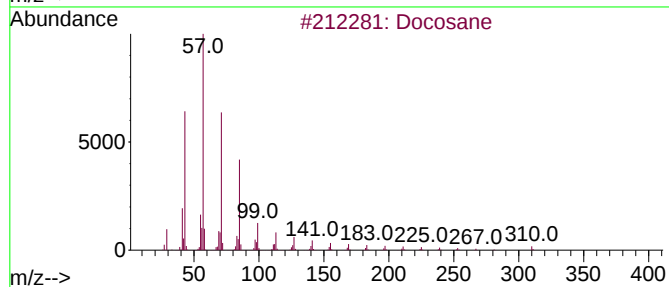
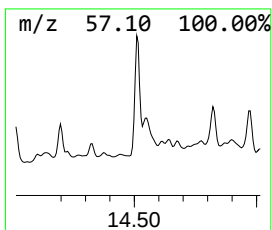
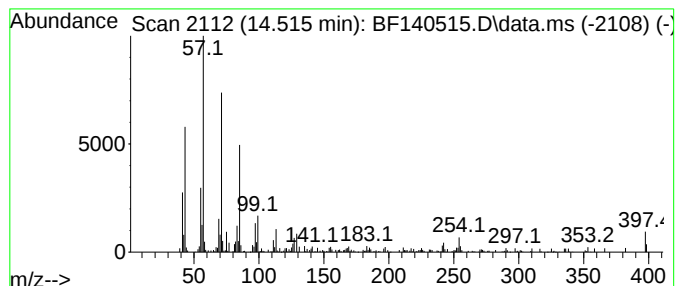
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	2.07 ng	89468	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	96
2			Tetracosane	338	C24H50	000646-31-1	93
3			Hexadecane	226	C16H34	000544-76-3	87
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83
5			Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
Operator : RC/JU
Sample : P4822-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SOIL-6

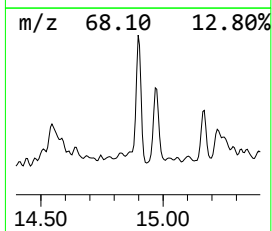
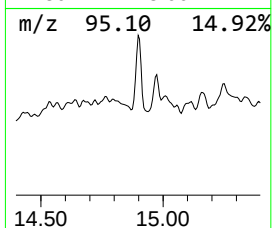
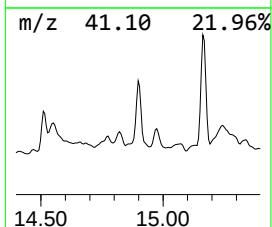
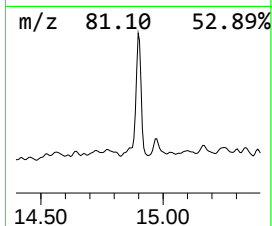
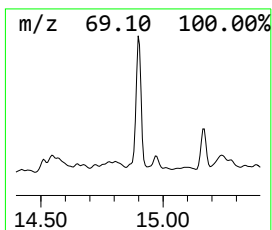
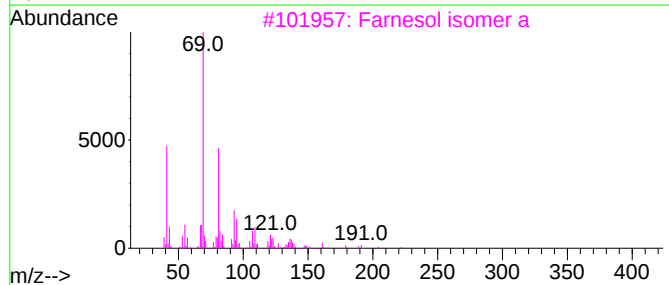
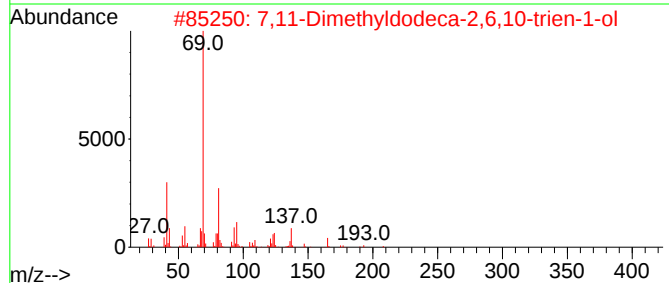
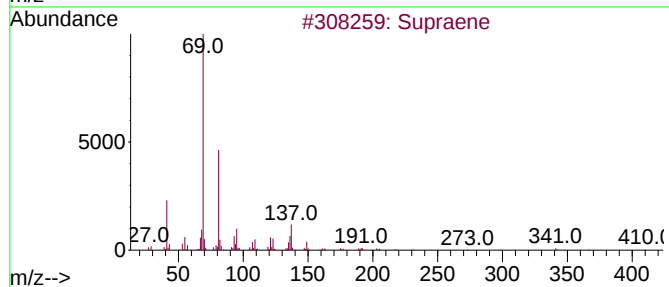
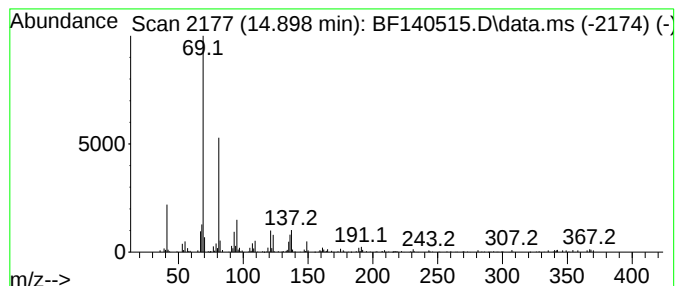
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	4.09 ng	112482	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3			Farnesol isomer a	222	C15H26O	1000108-92-4	64
4			Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
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ClientSampleId :
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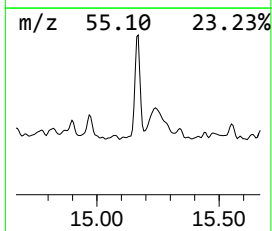
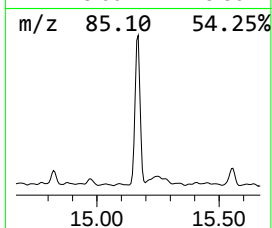
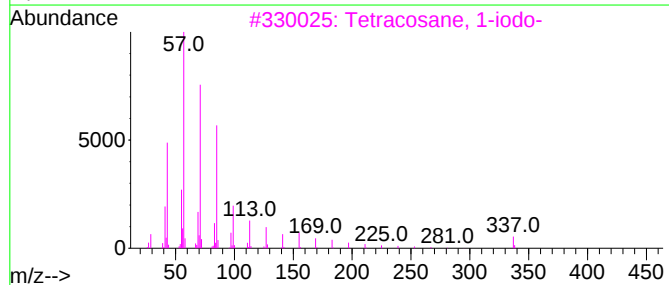
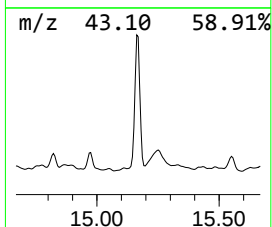
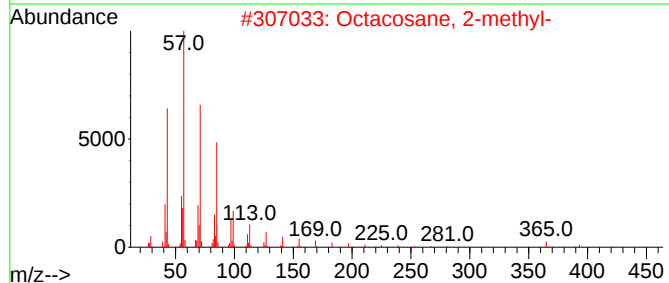
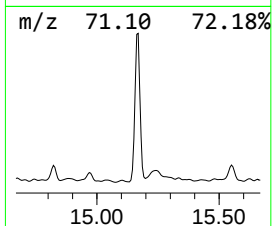
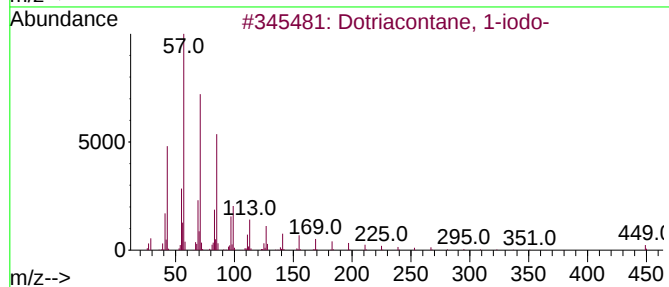
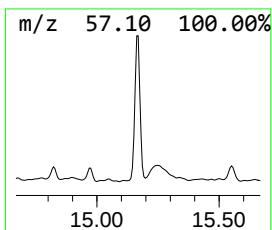
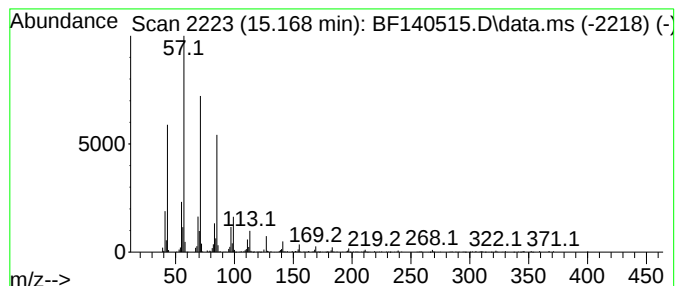
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dotriacontane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	11.07 ng	304191	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
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Misc :
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Instrument :
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ClientSampleId :
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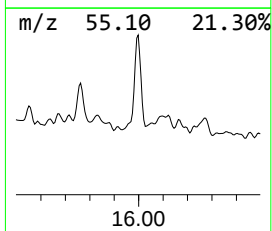
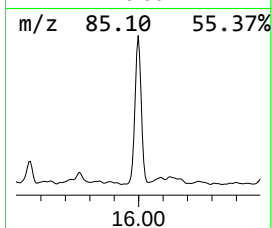
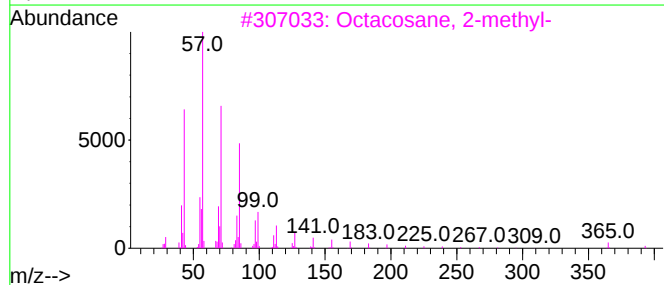
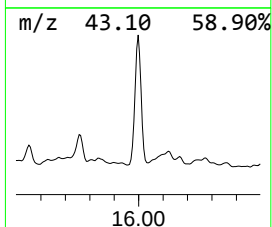
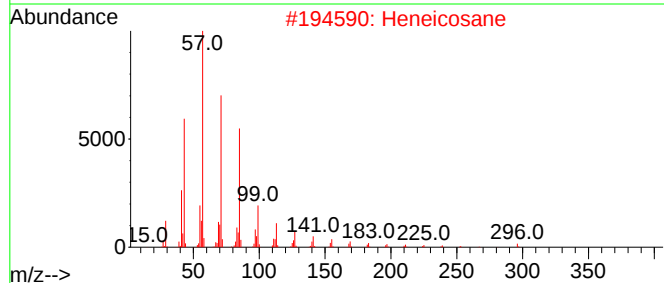
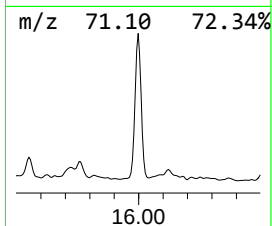
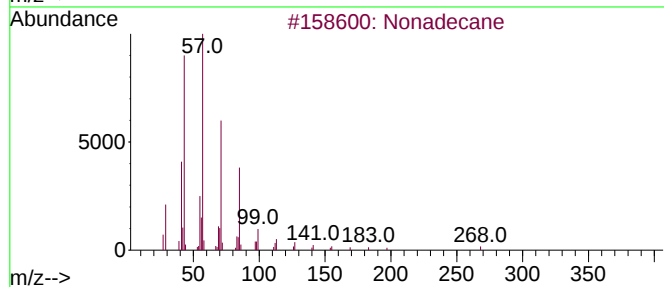
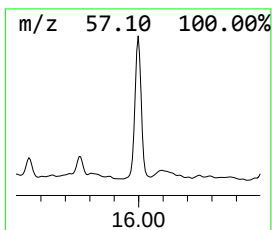
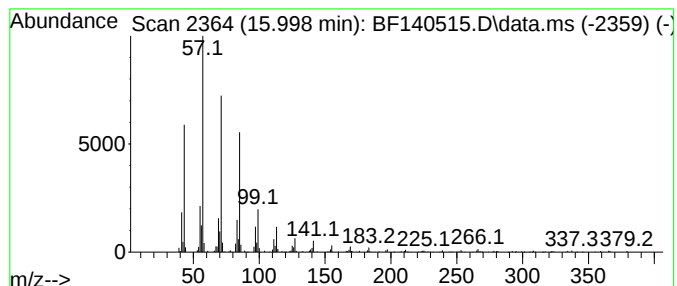
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	10.04 ng	275960	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	95
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
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ClientSampleId :
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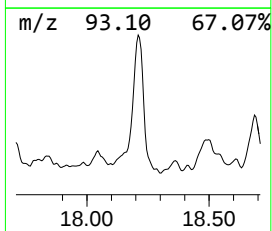
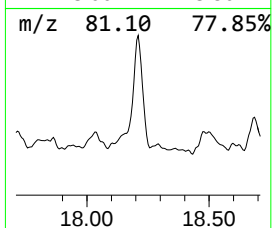
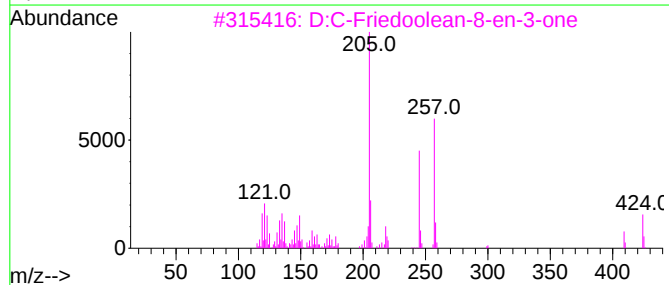
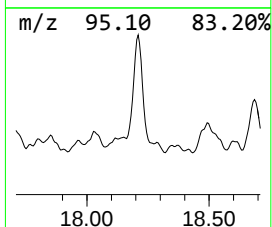
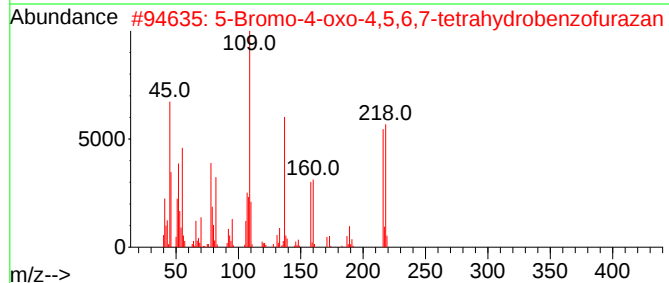
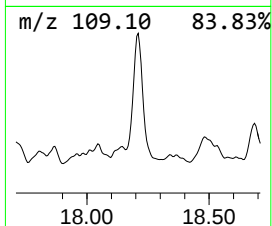
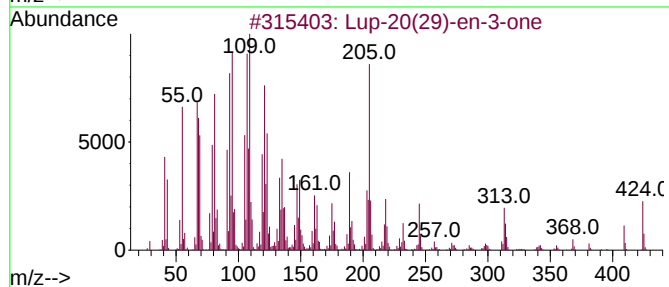
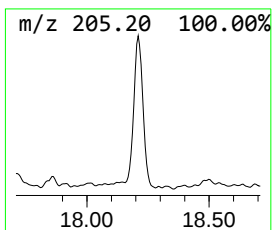
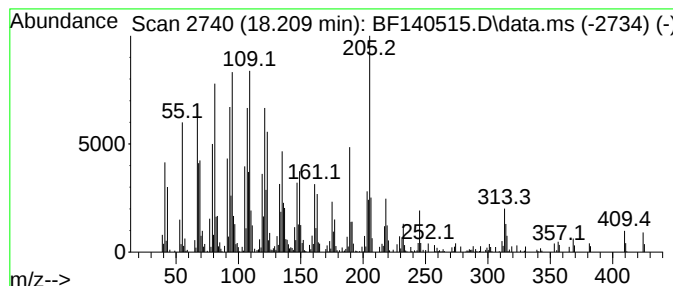
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	16.92 ng	465006	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
3			D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	74
4			2,6,6,9,2',6',6',9'-Octamethyl-[...]	410	C30H50	1000189-48-2	53
5			1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30O5	1000195-85-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
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ClientSampleId :
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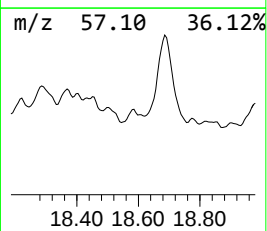
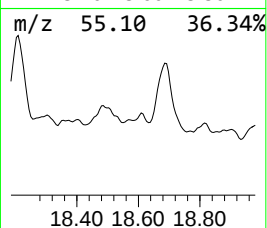
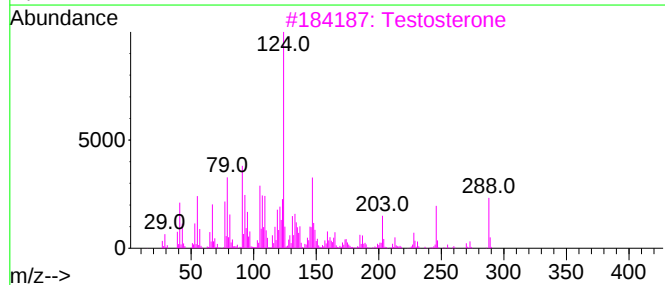
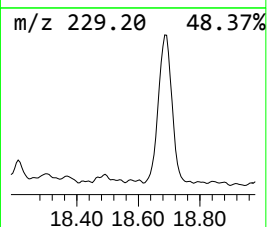
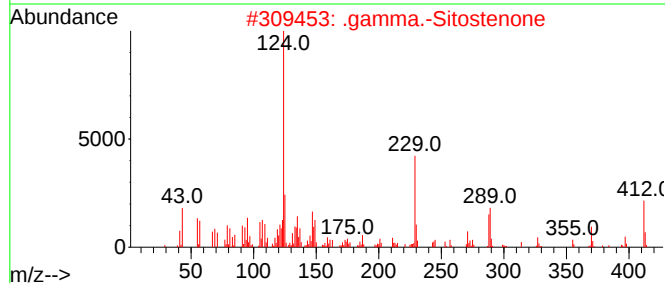
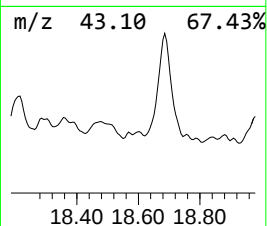
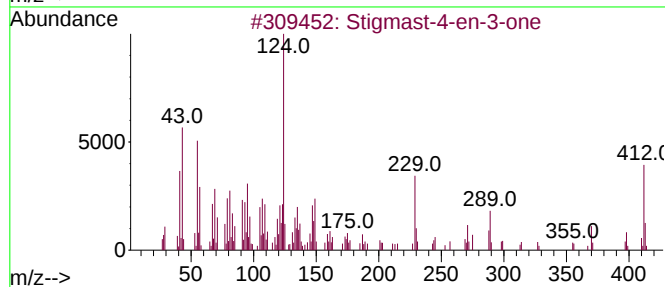
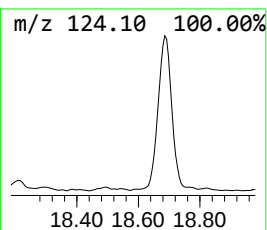
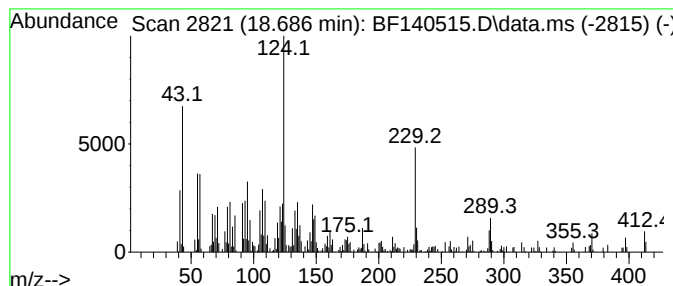
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Stigmast-4-en-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.686	14.56 ng	400307	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmast-4-en-3-one	412	C29H48O	001058-61-3	93
2			.gamma.-Sitostenone	412	C29H48O	084924-96-9	91
3			Testosterone	288	C19H28O2	000058-22-0	87
4			Testosterone cypionate	412	C27H40O3	000058-20-8	50
5			Cardoltriene	314	C21H30O2	079473-24-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140515.D
Acq On : 20 Nov 2024 22:13
Operator : RC/JU
Sample : P4822-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOIL-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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...	2.152	46.8	ng	1466270	1	6.875	627102	20.0
Benzophenone	10.622	13.6	ng	478134	3	9.910	701959	20.0
Methanone, (1-h...	10.927	2.1	ng	85012	4	11.398	812921	20.0
n-Hexadecanoic ...	11.922	14.1	ng	571498	4	11.398	812921	20.0
Octadecanoic acid	12.710	3.4	ng	139840	4	11.398	812921	20.0
1-Octadecene	13.886	5.5	ng	238982	5	14.045	865001	20.0
Docosane	14.515	2.1	ng	89468	5	14.045	865001	20.0
Supraene	14.898	4.1	ng	112482	6	15.545	549810	20.0
Dotriacontane, ...	15.168	11.1	ng	304191	6	15.545	549810	20.0
Nonadecane	15.998	10.0	ng	275960	6	15.545	549810	20.0
Lup-20(29)-en-3...	18.209	16.9	ng	465006	6	15.545	549810	20.0
Stigmast-4-en-3...	18.686	14.6	ng	400307	6	15.545	549810	20.0