

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
 Data File : BF140620.D
 Acq On : 25 Nov 2024 22:55
 Operator : RC/JU
 Sample : P4860-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PH2-BOT-003

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	504	509	520	rVB	22559	36099	2.20%	0.339%
2	5.493	573	578	600	rVB	924959	1254838	76.62%	11.779%
3	6.504	744	750	773	rBV	994270	1311890	80.10%	12.314%
4	6.869	807	812	821	rVB	288392	347691	21.23%	3.264%
5	7.428	902	907	920	rBV	630832	837662	51.15%	7.863%
6	8.151	1025	1030	1044	rBV	322172	428766	26.18%	4.025%
7	9.222	1207	1212	1223	rBV	1320324	1637791	100.00%	15.373%
8	9.904	1323	1328	1341	rBV	380756	484671	29.59%	4.549%
9	10.616	1444	1449	1457	rBV	78372	102573	6.26%	0.963%
10	10.698	1457	1463	1478	rBV	705269	967229	59.06%	9.079%
11	11.392	1576	1581	1590	rBV	385162	524003	31.99%	4.919%
12	11.916	1665	1670	1679	rBV	57249	96158	5.87%	0.903%
13	12.980	1845	1851	1856	rBV	1293919	1636377	99.91%	15.360%
14	13.545	1943	1947	1954	rBV5	8211	17501	1.07%	0.164%
15	13.904	2000	2008	2021	rBV6	22435	95499	5.83%	0.896%
16	14.010	2022	2026	2027	rVV	25739	30634	1.87%	0.288%
17	14.039	2027	2031	2048	rVB	277010	387992	23.69%	3.642%
18	14.880	2170	2174	2181	rVB	34165	47016	2.87%	0.441%
19	15.145	2216	2219	2225	rVB	14813	20609	1.26%	0.193%
20	15.527	2278	2284	2293	rBV	217145	348691	21.29%	3.273%
21	16.427	2433	2437	2445	rBV8	21896	39657	2.42%	0.372%

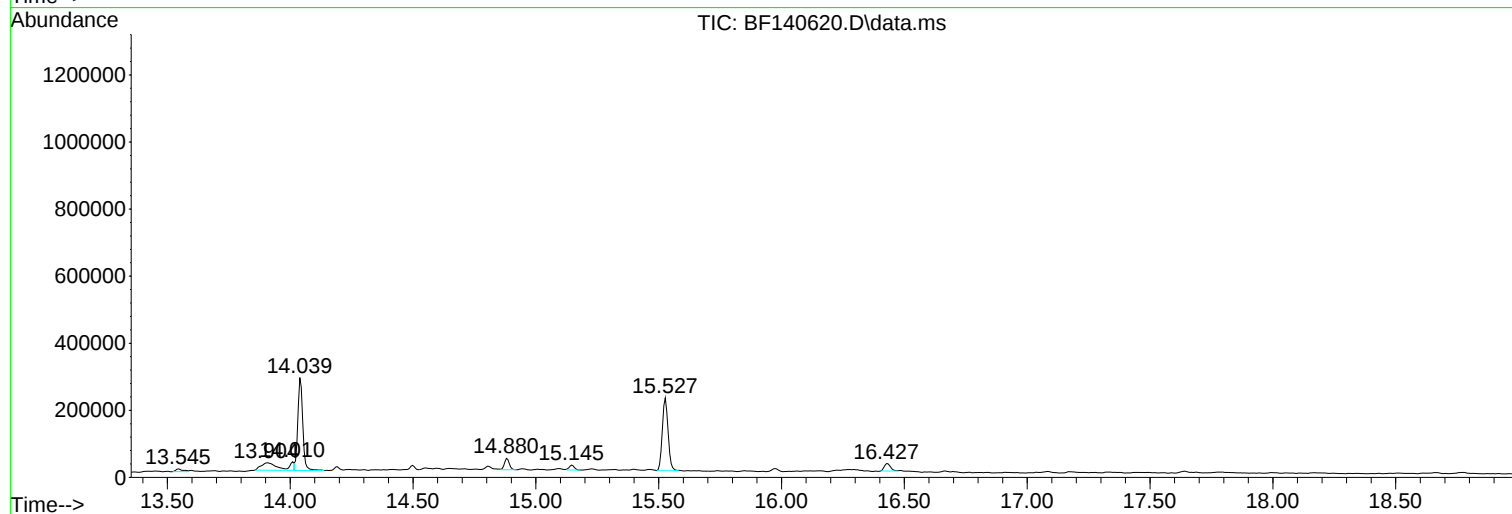
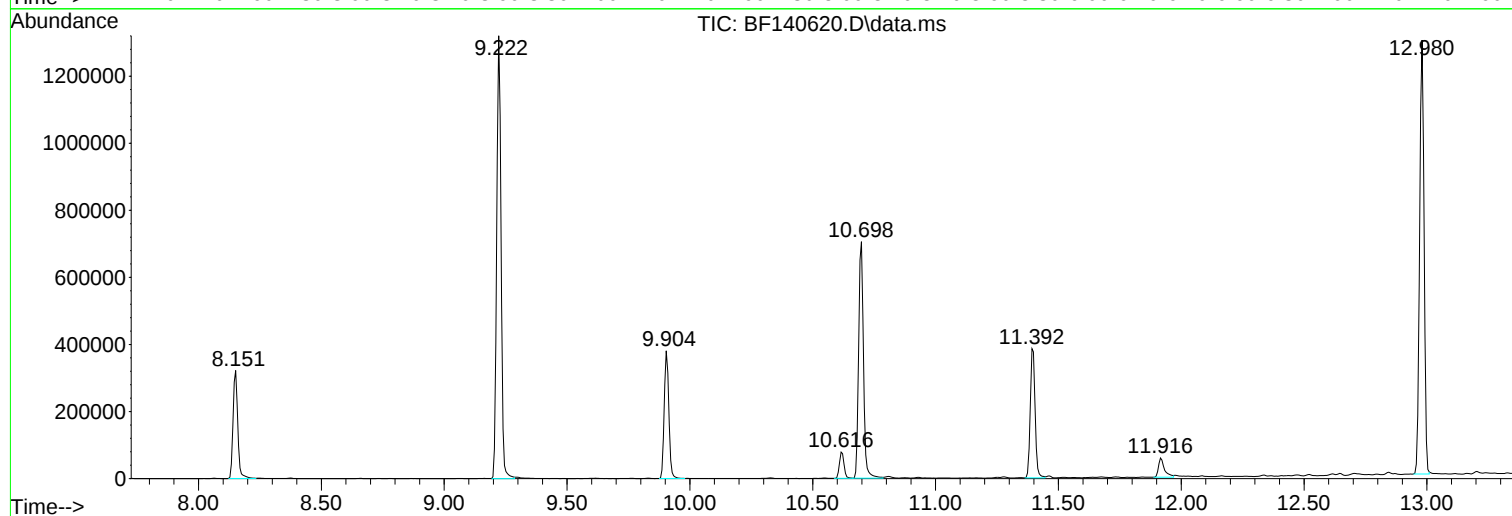
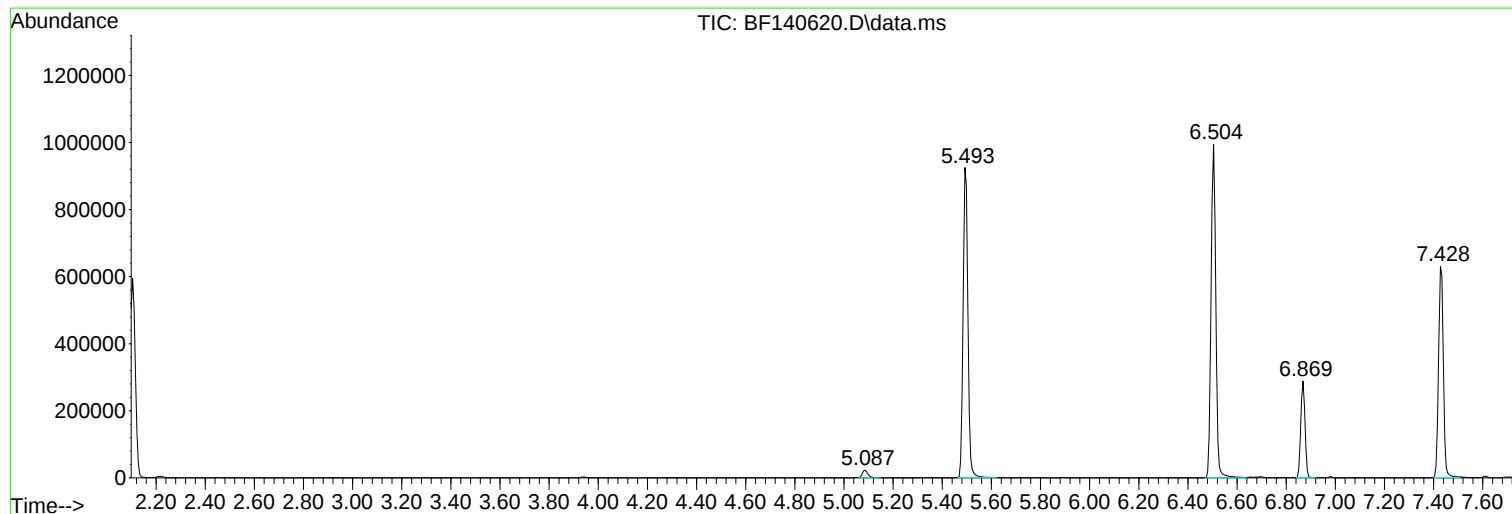
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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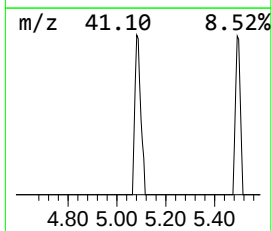
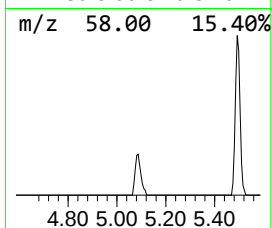
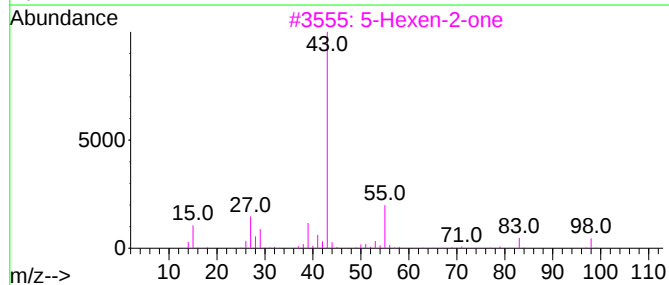
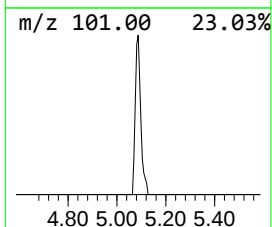
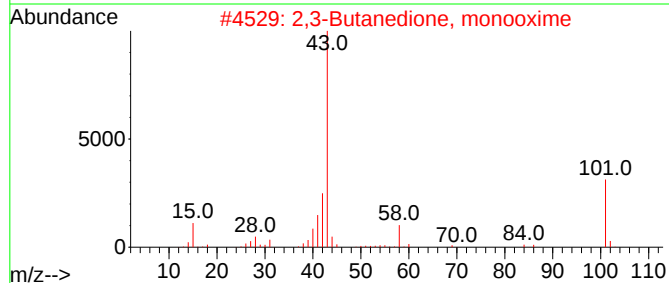
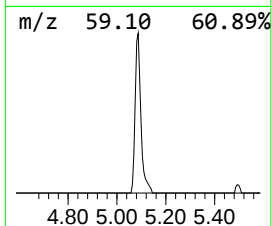
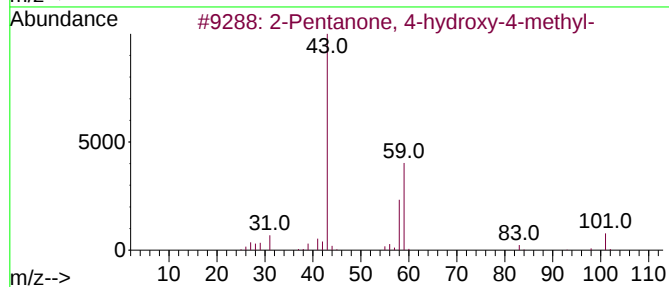
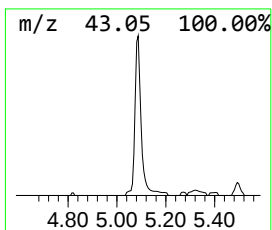
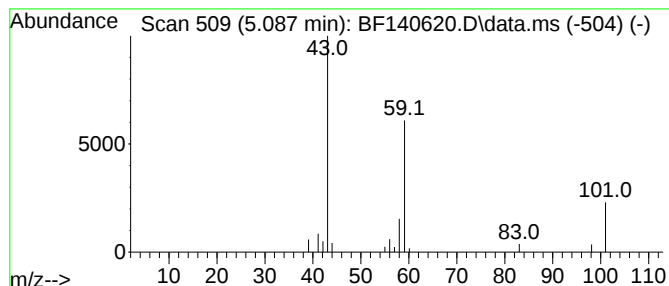
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.08 ng	36099	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		3-Octanol	130	C8H18O	000589-98-0	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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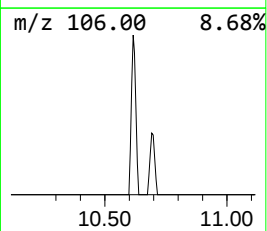
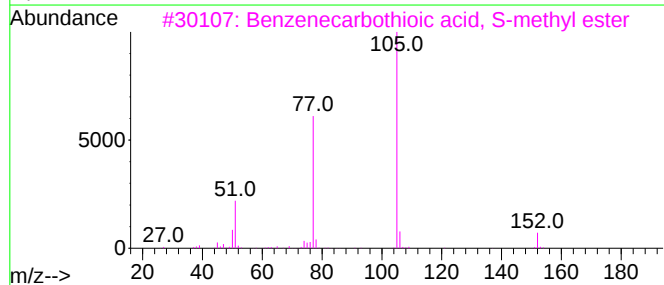
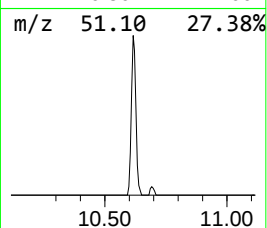
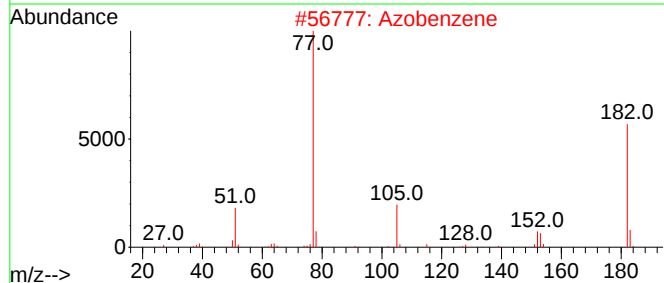
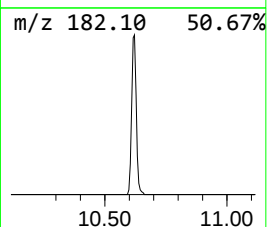
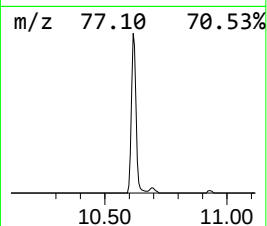
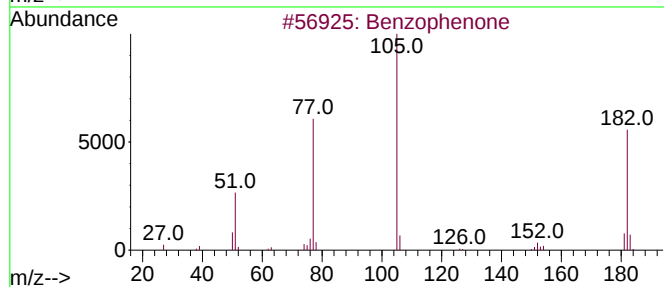
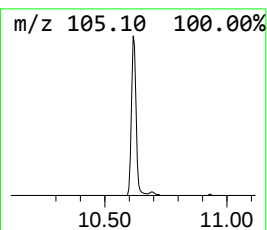
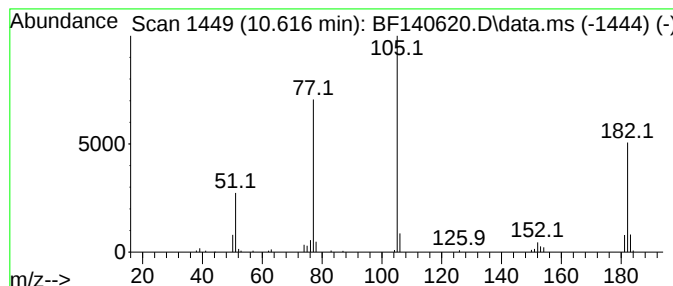
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	4.23 ng	102573	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



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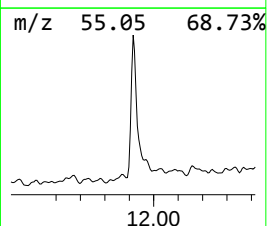
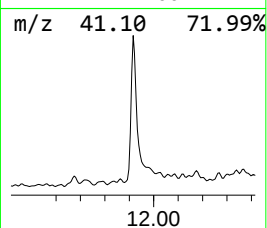
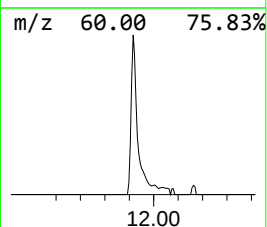
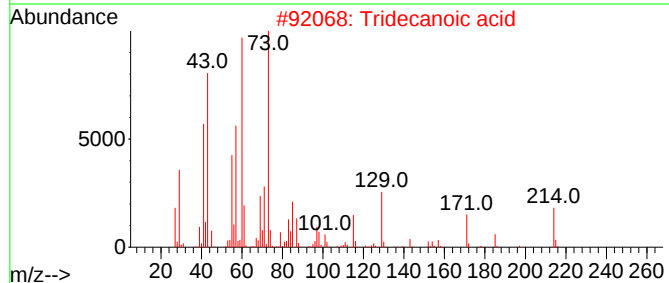
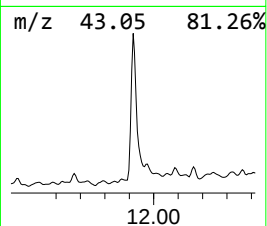
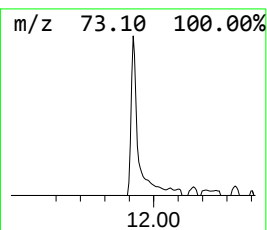
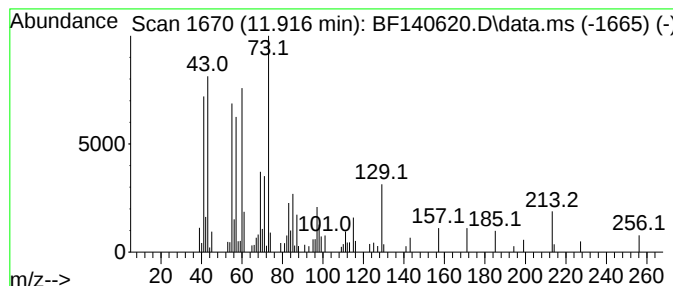
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.67 ng	96158	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



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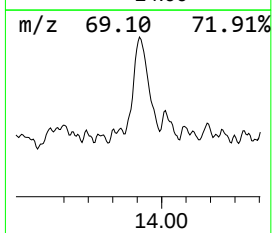
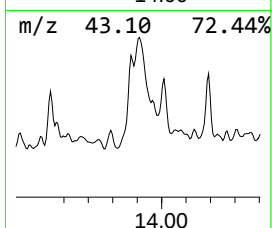
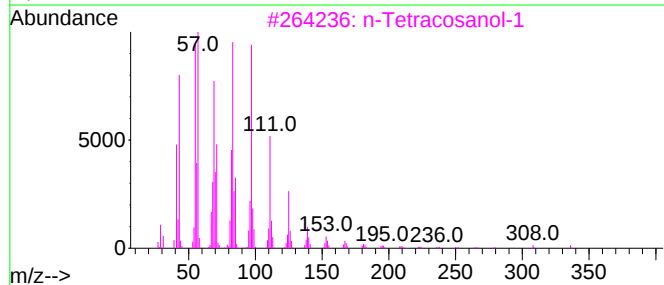
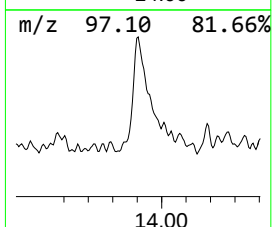
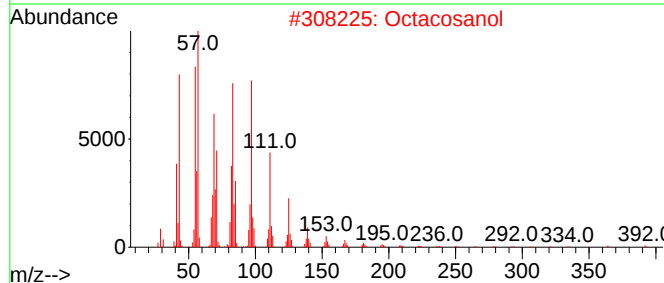
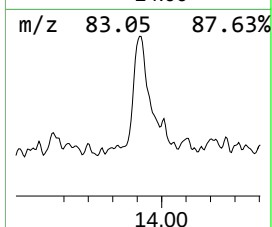
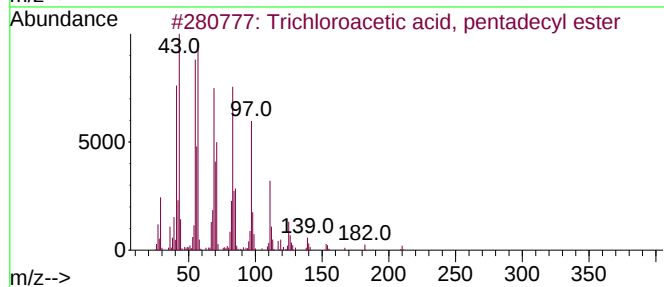
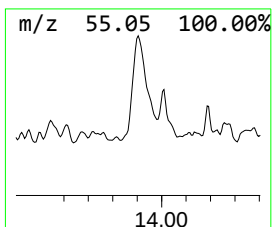
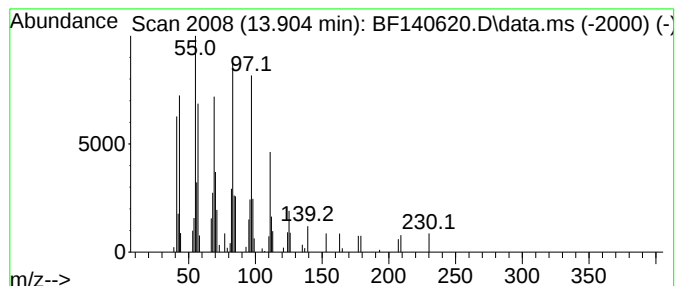
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.92 ng	95499	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2			Octacosanol	410	C28H58O	000557-61-9	87
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4			1-Tetracosene	336	C24H48	010192-32-2	87
5			1-Docosene	308	C22H44	001599-67-3	87



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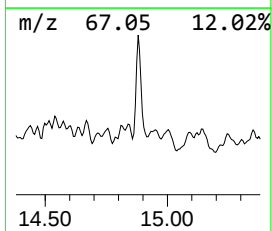
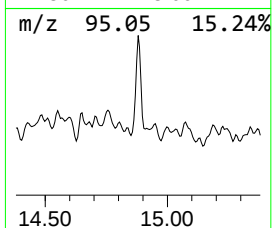
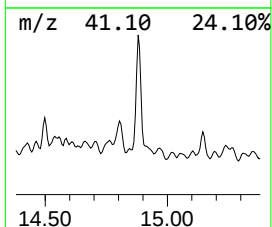
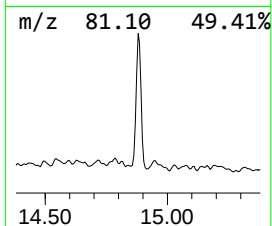
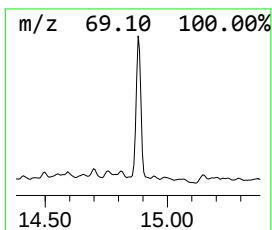
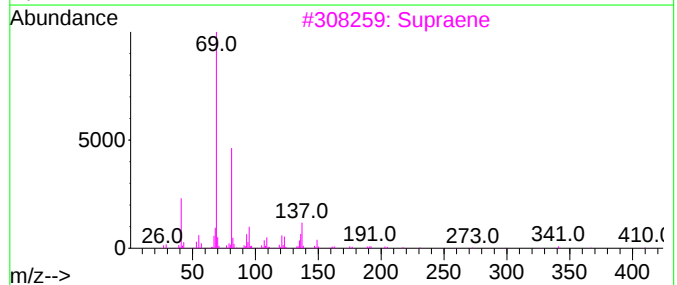
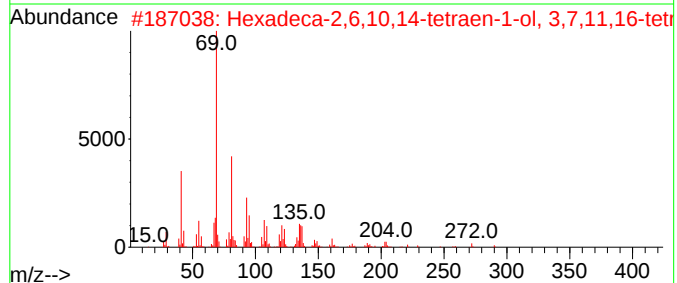
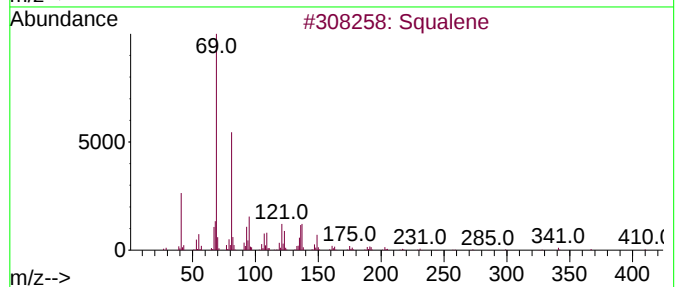
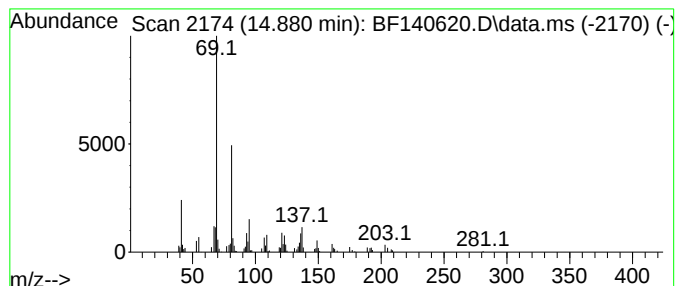
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.70 ng	47016	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	83
3			Supraene	410	C30H50	007683-64-9	83
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68



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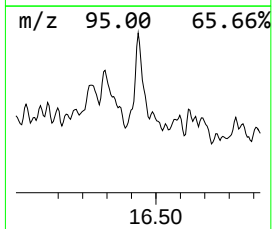
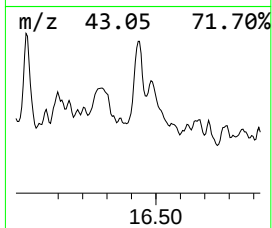
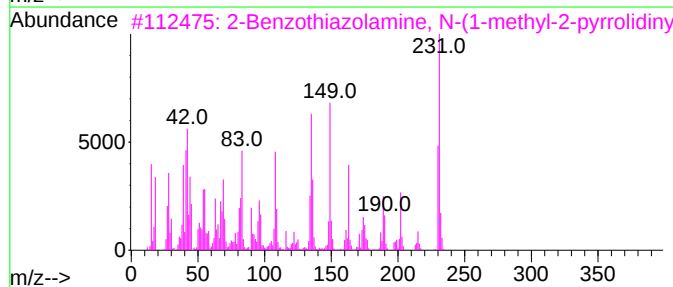
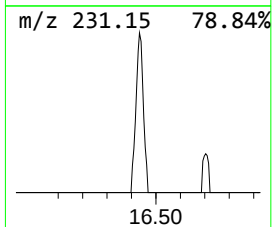
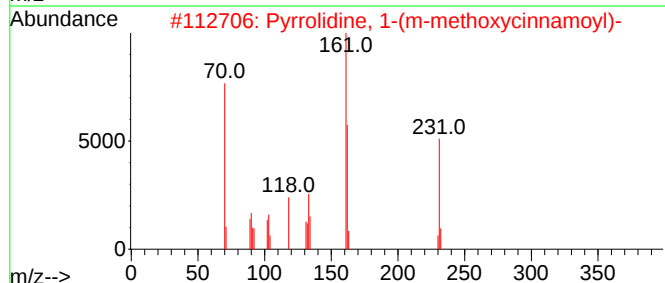
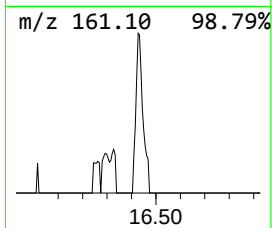
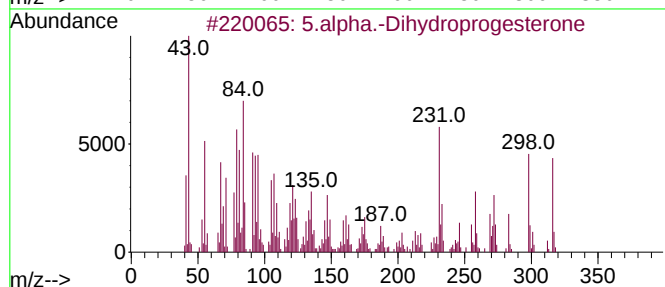
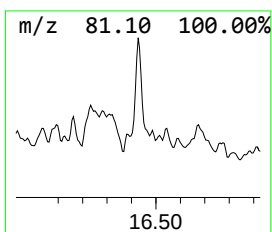
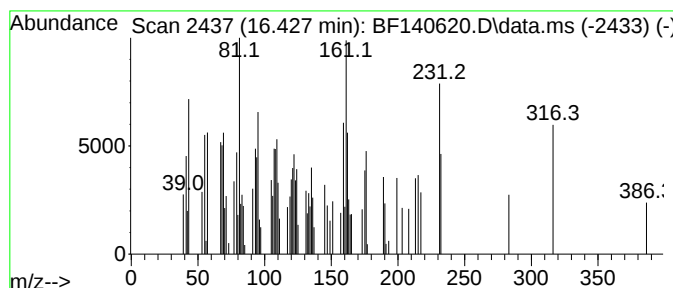
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.427 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.427	2.27 ng	39657	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.alpha.-Dihydroprogesterone	316	C21H32O2	000566-65-4	47		
2	Pyrrolidine, 1-(m-methoxycinnamo...	231	C14H17NO2	029647-01-6	35		
3	2-Benzothiazolamine, N-(1-methyl...	231	C12H13N3S	084859-07-4	25		
4	Pregn-5-en-20-one, 3-hydroxy-	316	C21H32O2	038372-24-6	25		
5	4-Methyl-2-(3-methyl-but-2-enyli...	176	C11H16N2	1000185-91-3	18		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112524\
Data File : BF140620.D
Acq On : 25 Nov 2024 22:55
Operator : RC/JU
Sample : P4860-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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
2-Pentanone, 4-...	5.087	2.1	ng	36099	1	6.869	347691	20.0
Benzophenone	10.616	4.2	ng	102573	3	9.904	484671	20.0
n-Hexadecanoic ...	11.916	3.7	ng	96158	4	11.392	524003	20.0
Trichloroacetic...	13.904	4.9	ng	95499	5	14.039	387992	20.0
Squalene	14.880	2.7	ng	47016	6	15.527	348691	20.0
unknown16.427	16.427	2.3	ng	39657	6	15.527	348691	20.0