

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128542.D
 Acq On : 28 May 2022 12:02
 Operator : CG\JU
 Sample : N2934-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P025-SS001-2430-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	469	473	480	rVB	133093	172952	3.18%	0.408%
2	5.457	533	539	542	rBV	4216534	4445453	81.74%	10.477%
3	6.463	704	710	713	rBV	3952326	4619794	84.94%	10.887%
4	6.575	726	729	733	rVB	99836	78320	1.44%	0.185%
5	6.840	770	774	777	rBV	1399972	1168554	21.49%	2.754%
6	7.398	864	869	872	rBV	2990690	3153579	57.98%	7.432%
7	8.116	987	991	995	rBV	1662971	1538882	28.29%	3.627%
8	9.198	1169	1175	1178	rBV	5427854	5438723	100.00%	12.817%
9	9.875	1284	1290	1294	rBV	2162679	1792364	32.96%	4.224%
10	10.663	1419	1424	1428	rBV	3431186	3597900	66.15%	8.479%
11	11.363	1539	1543	1546	rBV	2196267	1851307	34.04%	4.363%
12	11.763	1607	1611	1614	rVB	100754	89019	1.64%	0.210%
13	11.898	1626	1634	1656	rBV	1479500	1760373	32.37%	4.149%
14	12.169	1674	1680	1686	rVB3	51867	70319	1.29%	0.166%
15	12.598	1751	1753	1763	rVB3	40485	55872	1.03%	0.132%
16	12.686	1763	1768	1781	rBV	993235	1169165	21.50%	2.755%
17	12.957	1809	1814	1817	rBV	5213083	5210383	95.80%	12.279%
18	13.133	1841	1844	1848	rVB	140142	119459	2.20%	0.282%
19	13.321	1870	1876	1880	rBV	245315	253056	4.65%	0.596%
20	13.357	1880	1882	1888	rVV6	56525	86158	1.58%	0.203%
21	13.433	1891	1895	1900	rVB3	76937	90682	1.67%	0.214%
22	13.539	1907	1913	1917	rVB3	151313	202011	3.71%	0.476%
23	13.645	1927	1931	1934	rVB	162185	144278	2.65%	0.340%
24	13.827	1959	1962	1965	rBV	103687	93860	1.73%	0.221%
25	13.886	1965	1972	1986	rVV3	311448	1047566	19.26%	2.469%
26	14.004	1986	1992	1995	rVV	1542630	1514672	27.85%	3.570%
27	14.033	1995	1997	2001	rVV	222865	211383	3.89%	0.498%
28	14.098	2001	2008	2018	rVB	443002	497320	9.14%	1.172%
29	14.251	2031	2034	2038	rVB	107193	103922	1.91%	0.245%
30	14.545	2079	2084	2086	rBV6	30818	57097	1.05%	0.135%
31	14.868	2135	2139	2142	rBV	109652	111914	2.06%	0.264%
32	15.133	2180	2184	2187	rVB	62964	68488	1.26%	0.161%
33	15.462	2235	2240	2246	rBV	905687	1135896	20.89%	2.677%
34	15.951	2319	2323	2328	rVB	62435	86193	1.58%	0.203%
35	16.098	2339	2348	2359	rBV7	60368	235537	4.33%	0.555%
36	17.286	2545	2550	2560	rVB7	70681	159762	2.94%	0.377%

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ClientSampleId :
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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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

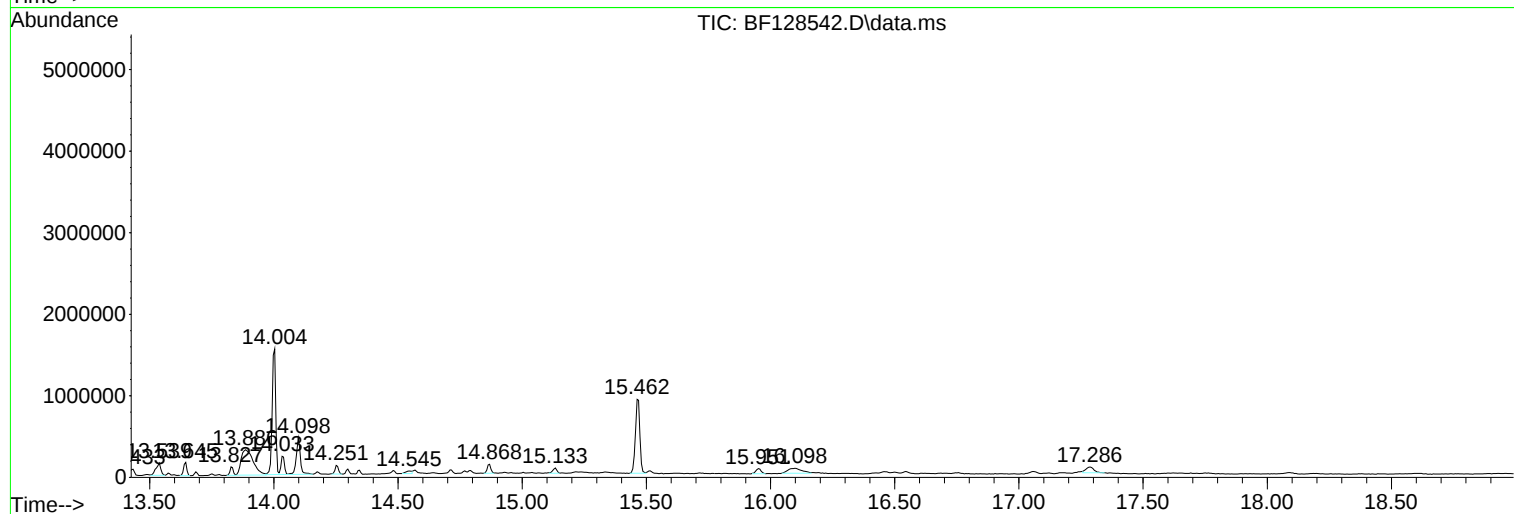
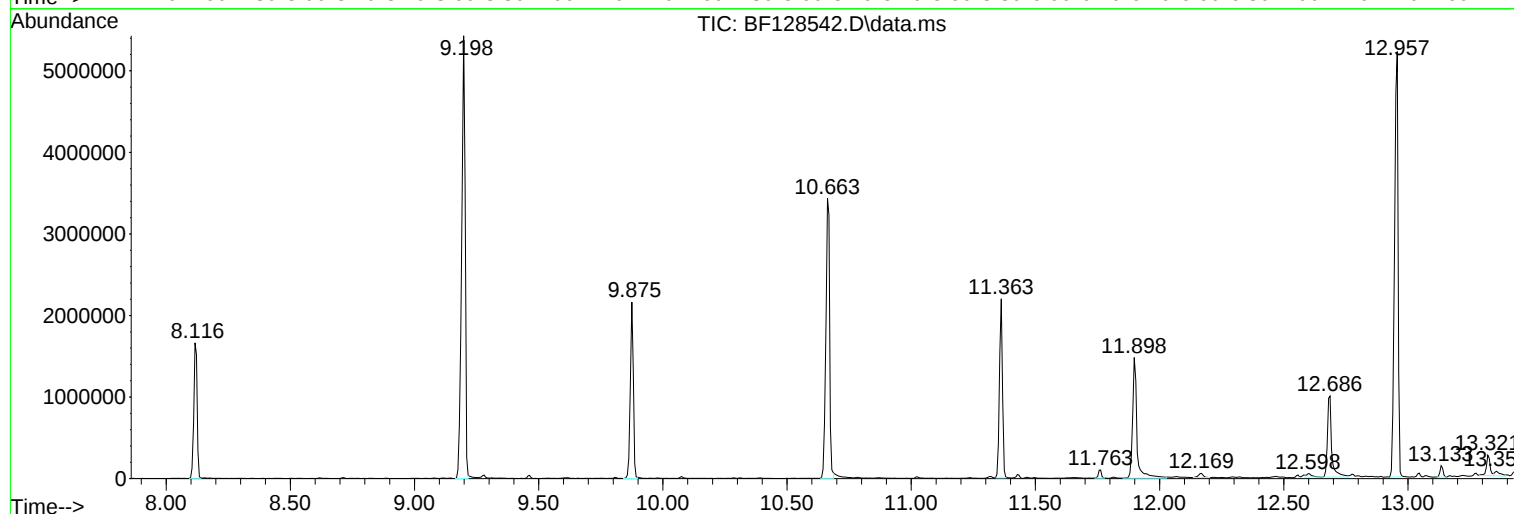
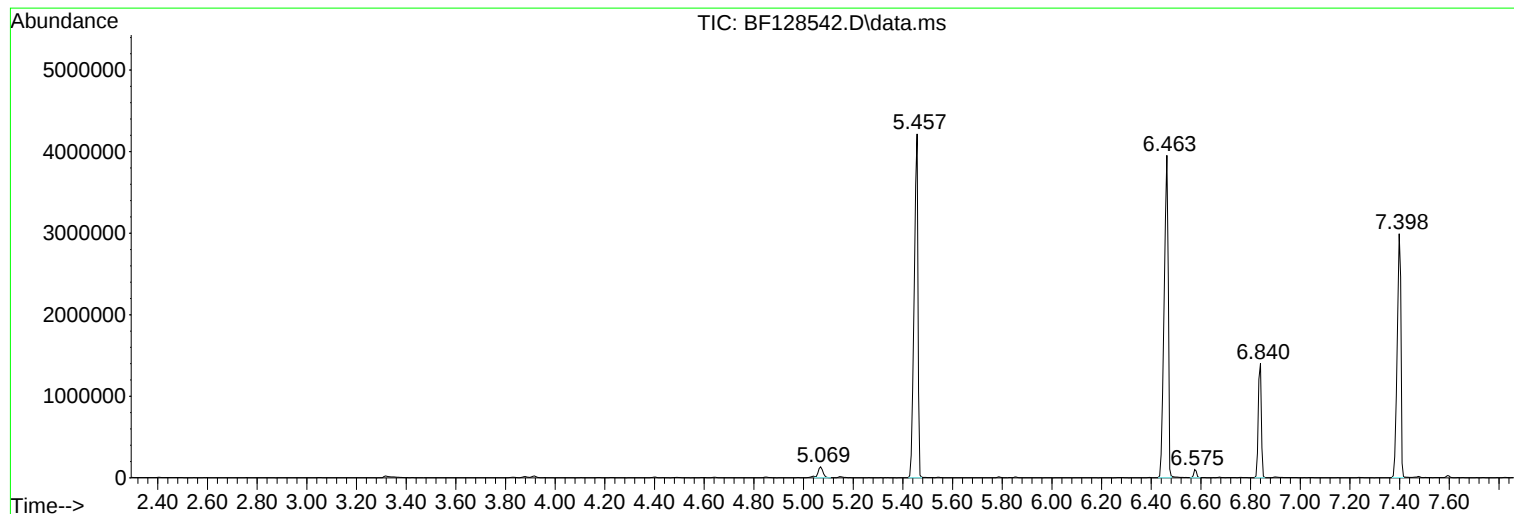
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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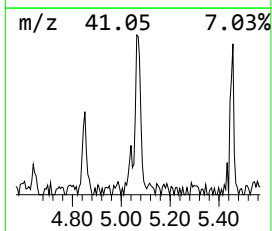
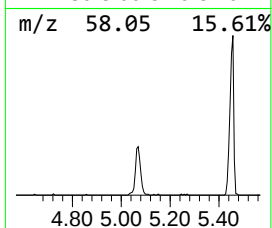
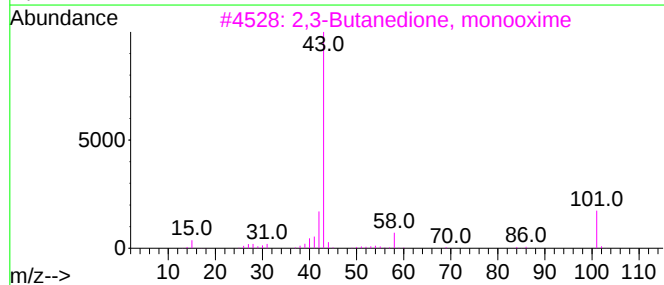
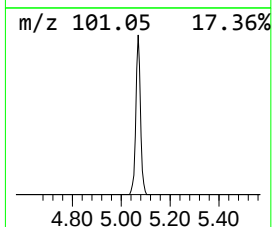
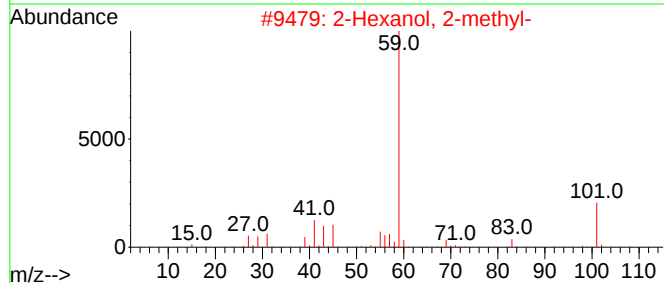
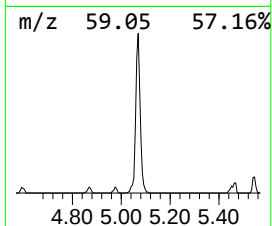
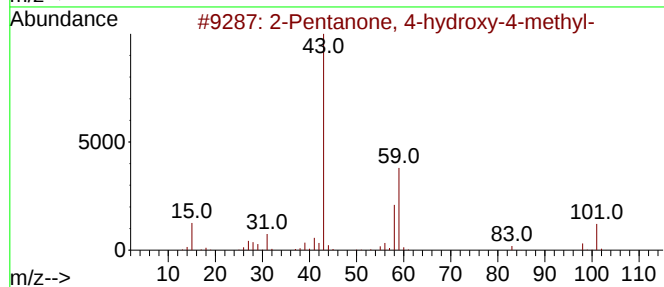
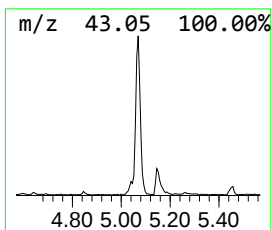
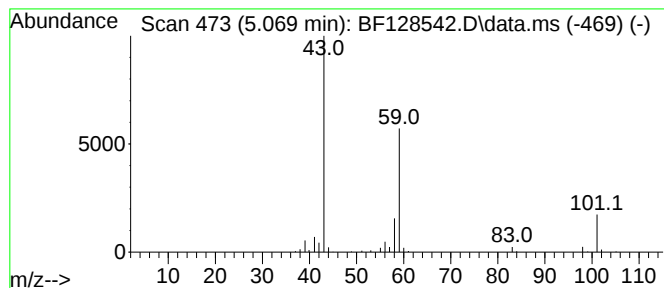
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.069	2.96 ng	172952	1,4-Dichlorobenzene-d4			6.840
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12



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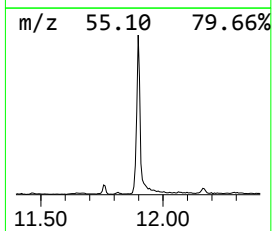
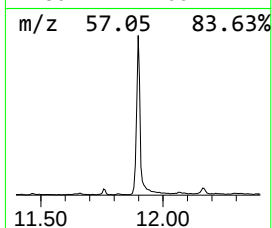
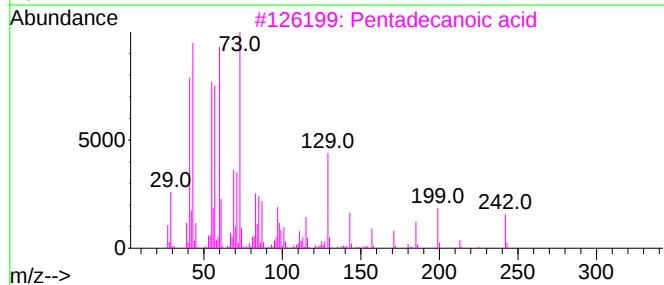
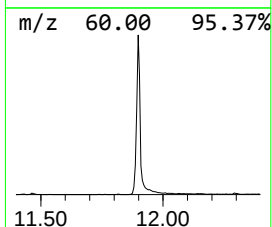
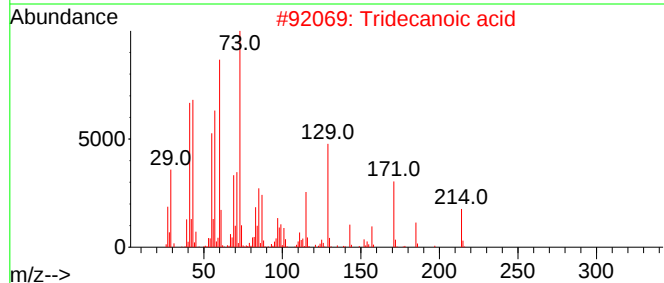
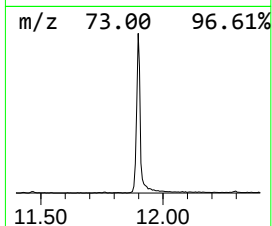
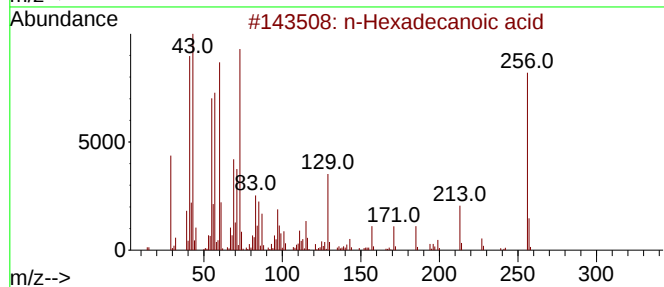
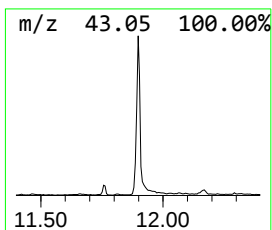
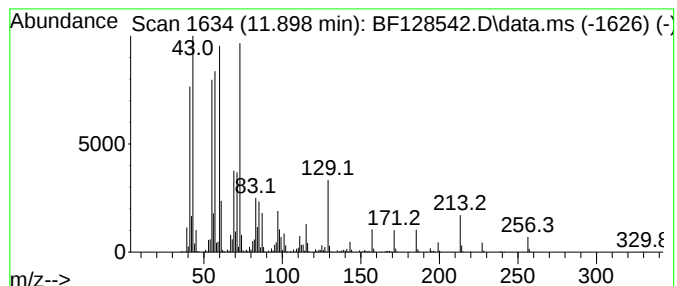
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.898	19.02 ng	1760370	Phenanthrene-d10		11.363	
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	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Undecanoic acid		186	C11H22O2	000112-37-8	68



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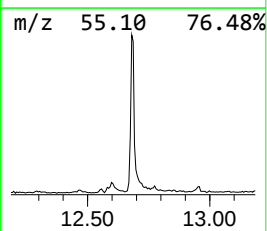
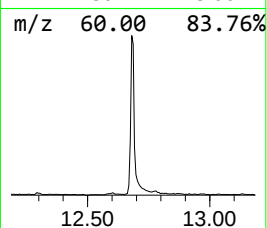
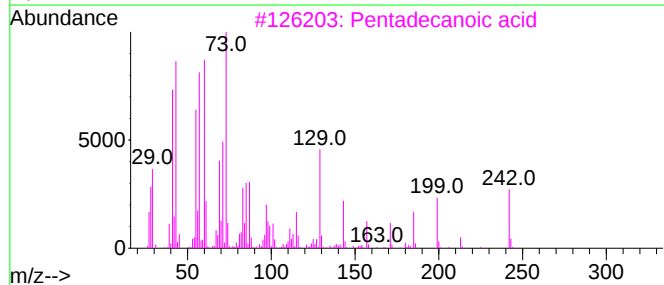
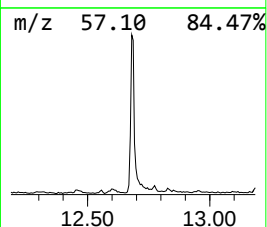
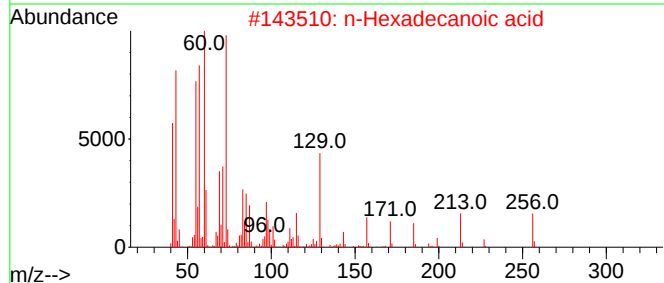
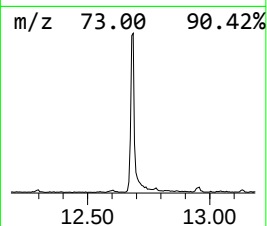
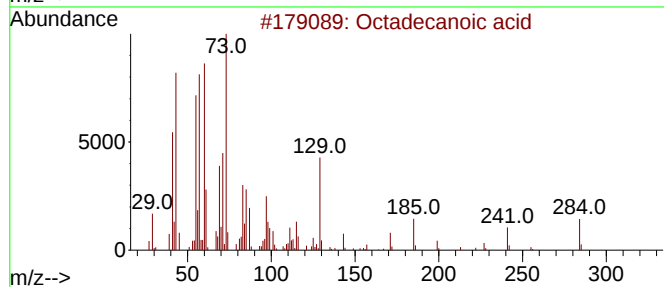
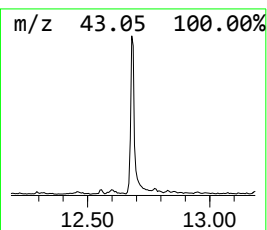
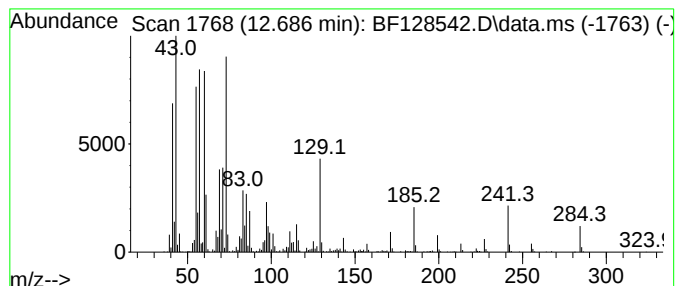
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	15.44 ng	1169170	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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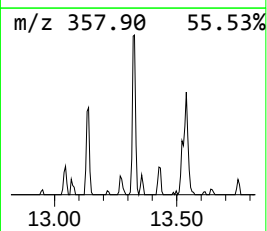
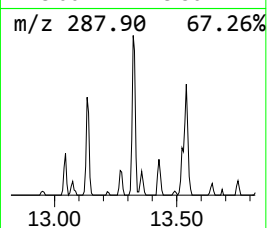
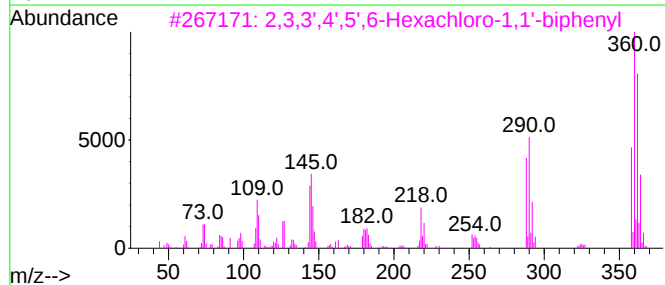
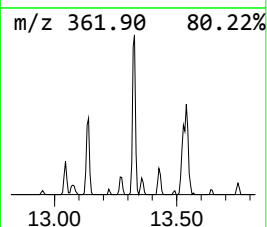
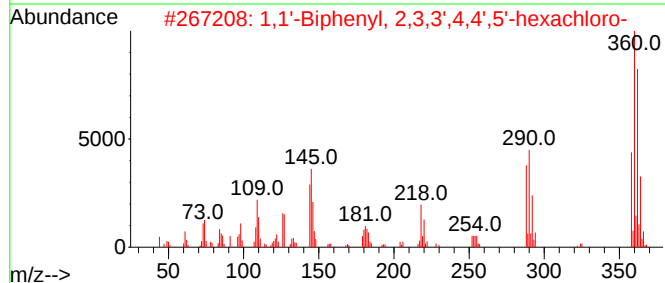
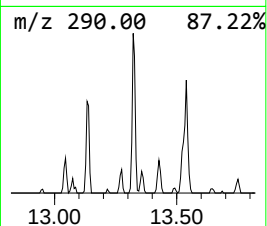
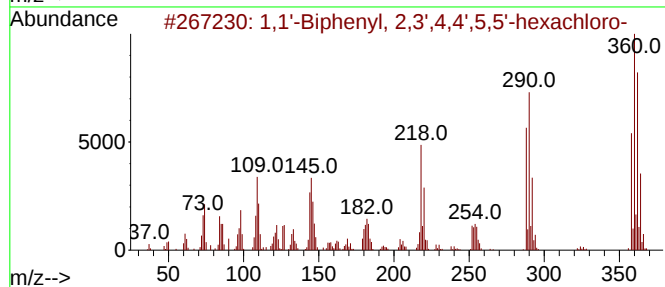
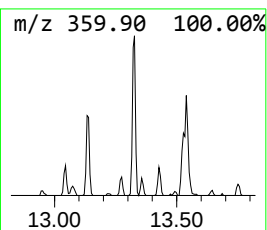
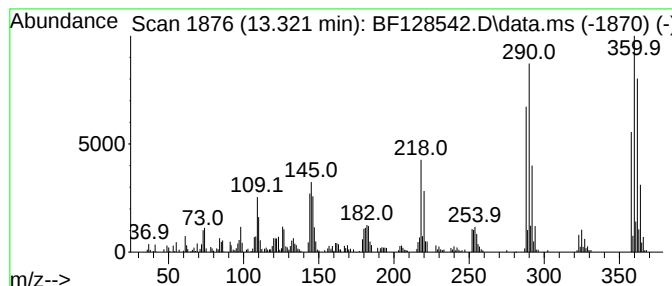
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 2,3',4,4',5,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	3.34 ng	253056	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,3',4,4',5,5'-he...	358	C12H4Cl6	052663-72-6	99		
2	1,1'-Biphenyl, 2,3,3',4,4',5'-he...	358	C12H4Cl6	069782-90-7	99		
3	2,3,3',4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	074472-45-0	99		
4	2,2',3,4,6,6'-Hexachloro-1,1'-bi...	358	C12H4Cl6	074472-40-5	99		
5	2,3',4,4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	059291-65-5	99		



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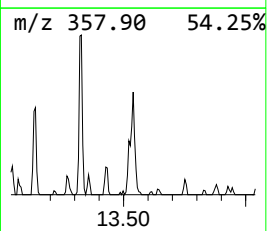
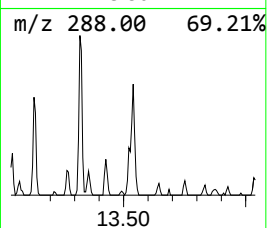
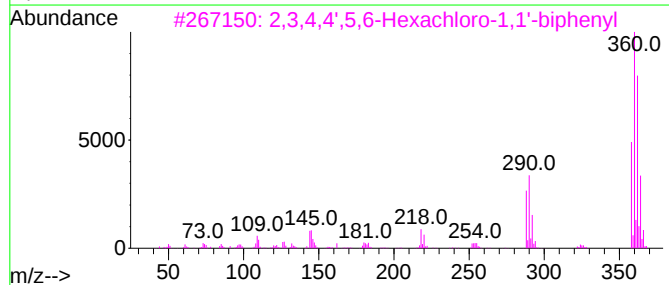
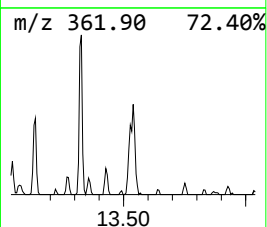
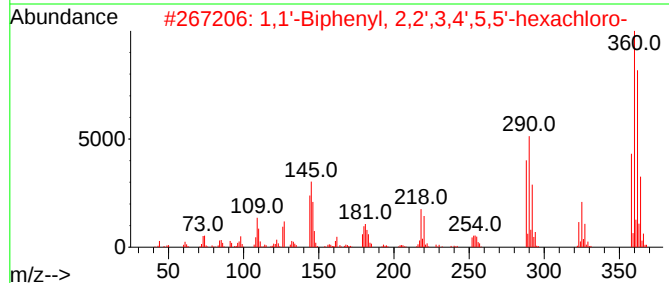
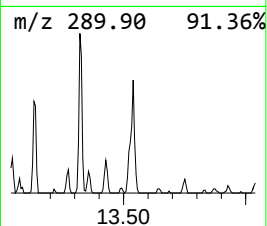
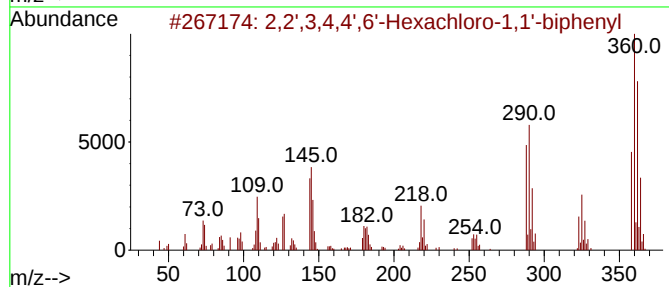
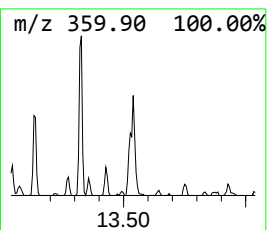
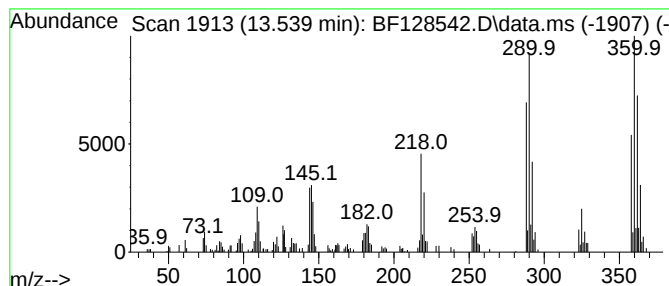
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2,2',3,4,4',6'-Hexachloro-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.539	2.67 ng	202011	Chrysene-d12		14.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,2',3,4,4',6'-Hexachloro-1,1'-b...		358	C12H4Cl6	059291-64-4	99
2	1,1'-Biphenyl, 2,2',3,4',5,5'-he...		358	C12H4Cl6	051908-16-8	99
3	2,3,4,4',5,6-Hexachloro-1,1'-bip...		358	C12H4Cl6	041411-63-6	99
4	2,3,3',4',5',6-Hexachloro-1,1'-b...		358	C12H4Cl6	074472-45-0	99
5	2,2',3,5,6,6'-Hexachloro-1,1'-bi...		358	C12H4Cl6	068194-09-2	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128542.D
Acq On : 28 May 2022 12:02
Operator : CG\JU
Sample : N2934-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

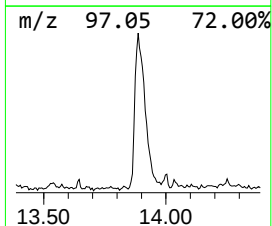
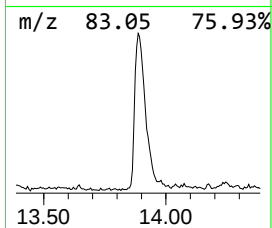
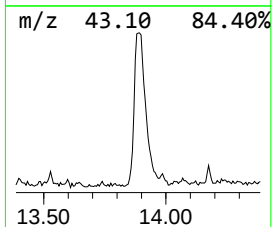
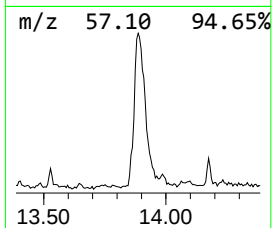
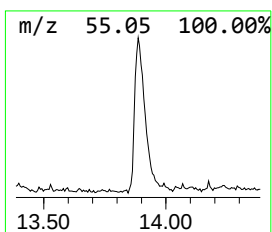
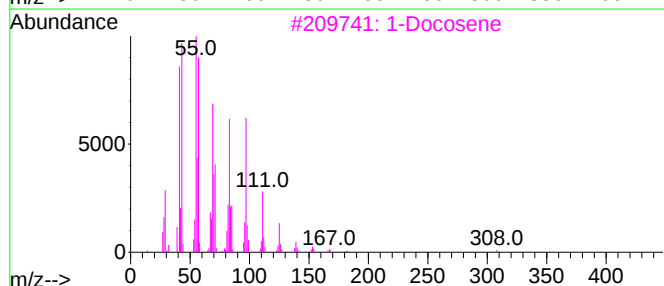
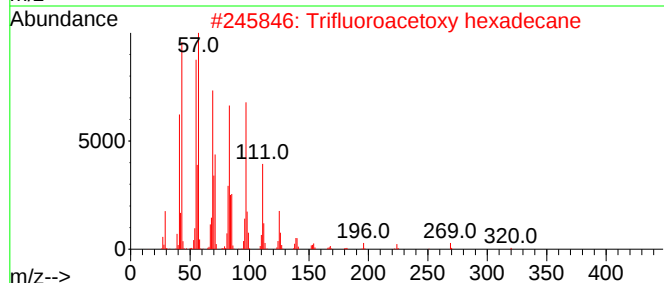
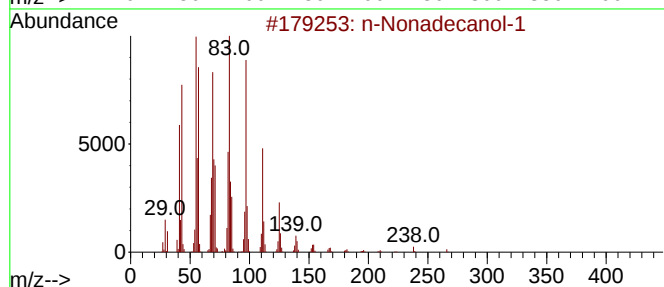
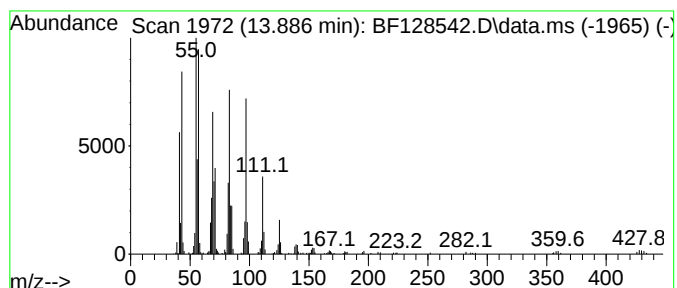
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ClientSampleId :
P025-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	13.83 ng	1047570	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128542.D
Acq On : 28 May 2022 12:02
Operator : CG\JU
Sample : N2934-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P025-SS001-2430-01

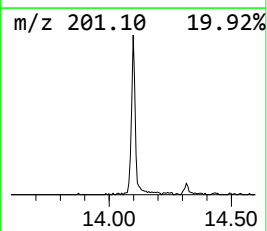
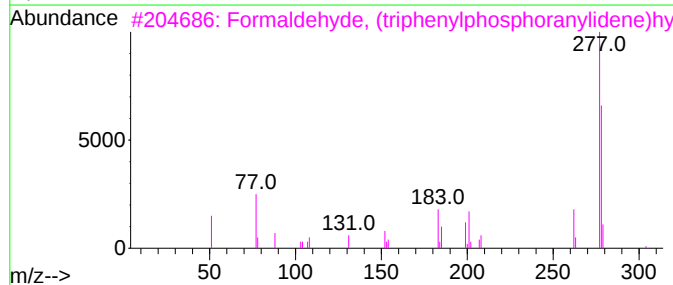
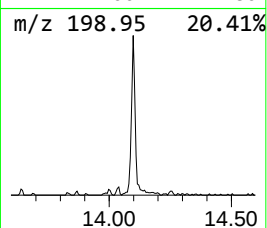
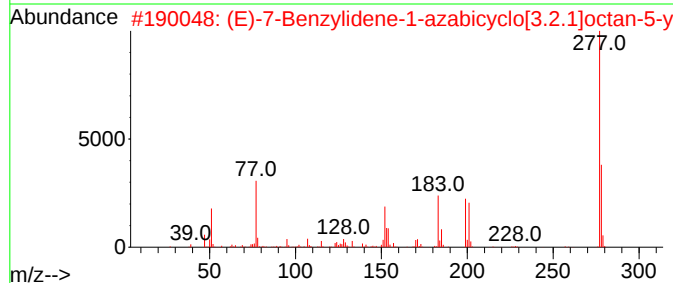
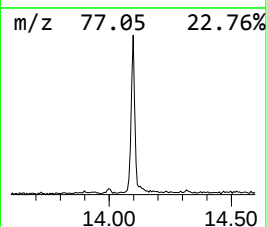
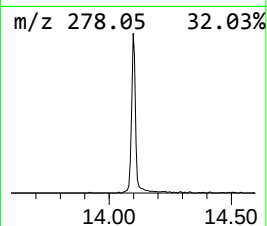
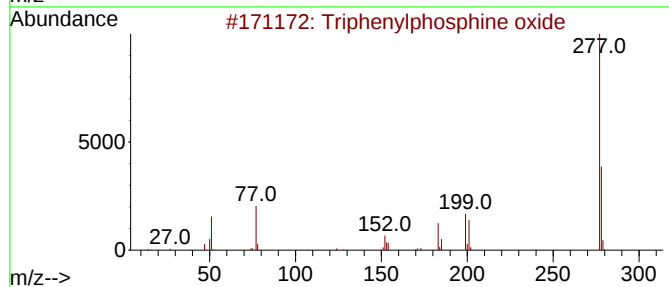
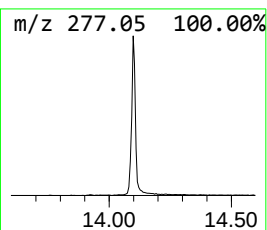
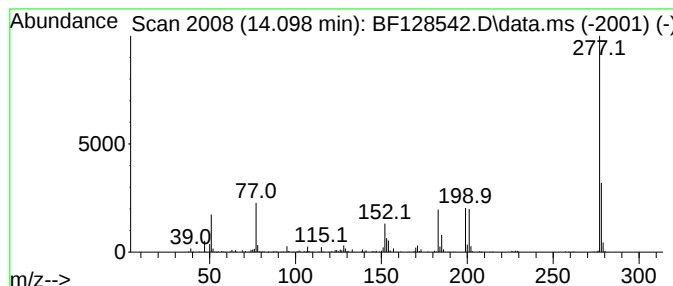
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	6.57 ng	497320	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128542.D
Acq On : 28 May 2022 12:02
Operator : CG\JU
Sample : N2934-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P025-SS001-2430-01

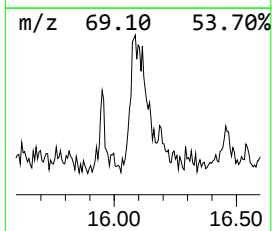
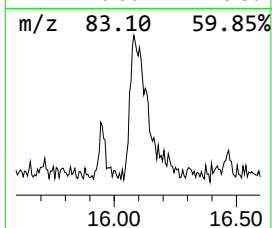
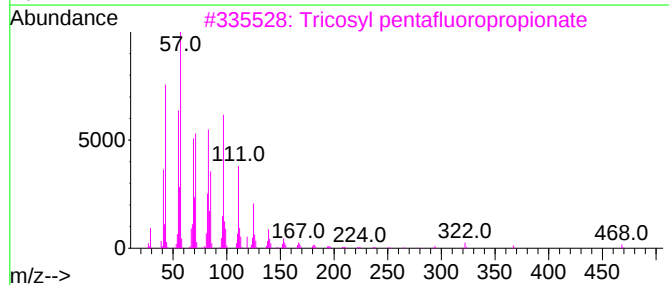
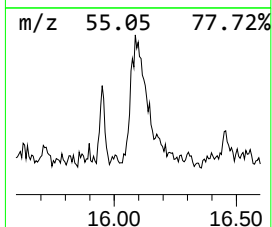
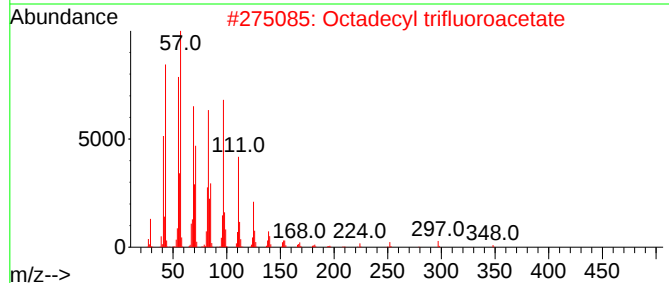
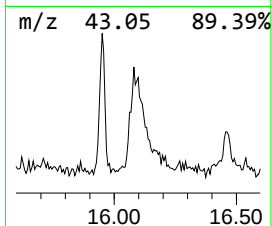
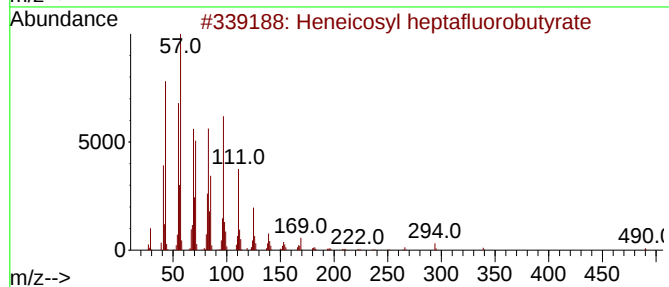
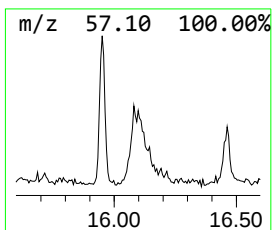
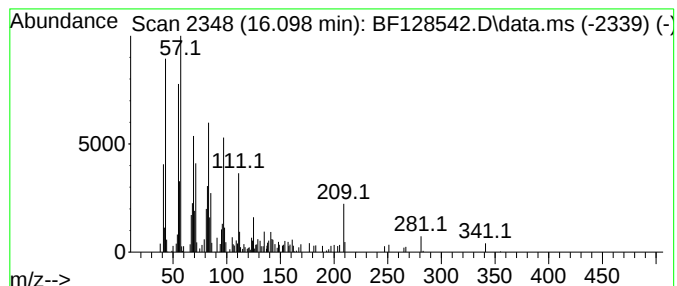
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	4.15 ng	235537	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	81
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	81
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	81
5			Octacosanol	410	C28H58O	000557-61-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128542.D
Acq On : 28 May 2022 12:02
Operator : CG\JU
Sample : N2934-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P025-SS001-2430-01

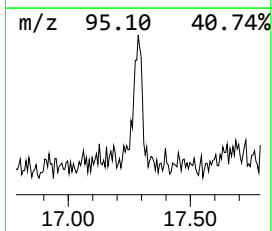
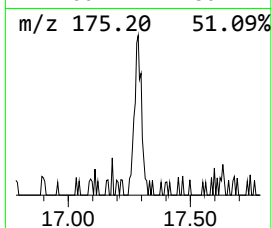
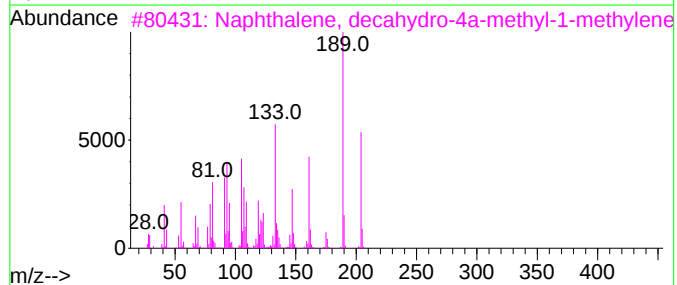
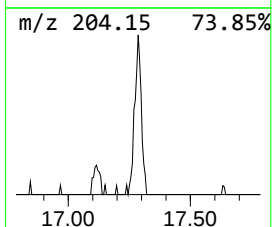
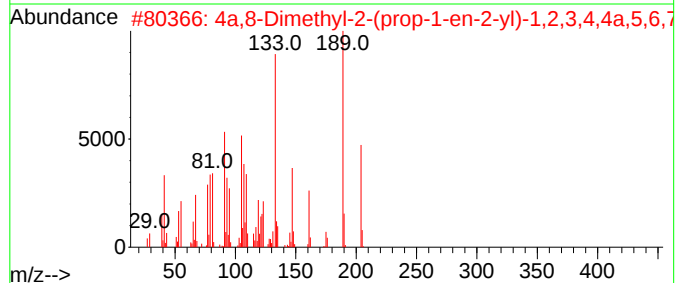
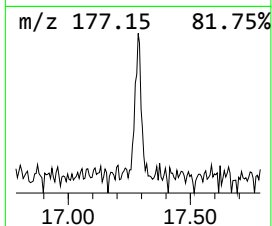
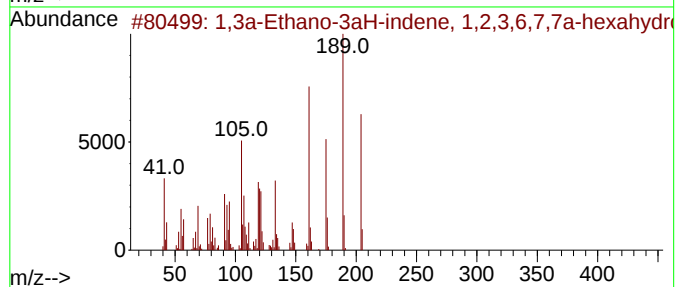
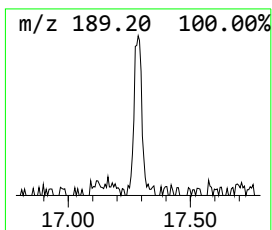
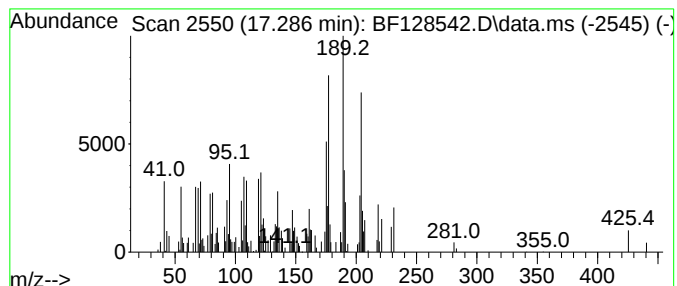
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3a-Ethano-3aH-indene, 1,2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	2.81 ng	159762	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	70
2			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	64
3			Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	46
4			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	38
5			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128542.D
Acq On : 28 May 2022 12:02
Operator : CG\JU
Sample : N2934-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P025-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
2-Pentanone, 4-...	5.069	3.0	ng	172952	1	6.840	1168550	20.0
n-Hexadecanoic ...	11.898	19.0	ng	1760370	4	11.363	1851310	20.0
Octadecanoic acid	12.686	15.4	ng	1169170	5	14.004	1514670	20.0
1,1'-Biphenyl, ...	13.322	3.3	ng	253056	5	14.004	1514670	20.0
2,2',3,4,4',6'-...	13.539	2.7	ng	202011	5	14.004	1514670	20.0
n-Nonadecanol-1	13.886	13.8	ng	1047570	5	14.004	1514670	20.0
Triphenylphosph...	14.098	6.6	ng	497320	5	14.004	1514670	20.0
Heneicosyl hept...	16.098	4.2	ng	235537	6	15.468	1135900	20.0
1,3a-Ethano-3aH...	17.286	2.8	ng	159762	6	15.468	1135900	20.0