

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
 Data File : BF128674.D
 Acq On : 03 Jun 2022 12:17
 Operator : CG\JU
 Sample : N2987-15
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P027-SS004-0006-01

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	465	469	474	rVB	24466	31333	1.03%	0.155%
2	5.469	538	541	559	rVB	2419076	2446268	80.65%	12.107%
3	6.481	710	713	724	rBV	2358735	2475091	81.60%	12.249%
4	6.822	767	771	774	rVB	746863	578791	19.08%	2.864%
5	7.387	861	867	870	rBV	1811107	1706071	56.24%	8.443%
6	8.104	984	989	992	rBV	889966	735887	24.26%	3.642%
7	9.187	1167	1173	1176	rBV	3041914	3033366	100.00%	15.012%
8	9.863	1283	1288	1291	rBV	926326	840929	27.72%	4.162%
9	10.657	1417	1423	1426	rBV	2171230	2069586	68.23%	10.242%
10	11.351	1536	1541	1544	rBV	913859	850615	28.04%	4.210%
11	11.880	1625	1631	1639	rBV	295264	290243	9.57%	1.436%
12	12.022	1651	1655	1662	rBV3	44686	70343	2.32%	0.348%
13	12.098	1662	1668	1679	rVB6	40025	118345	3.90%	0.586%
14	12.663	1759	1764	1773	rBV	112498	136643	4.50%	0.676%
15	12.939	1806	1811	1814	rBV	3201451	2726646	89.89%	13.494%
16	13.886	1966	1972	1985	rVV3	87499	262101	8.64%	1.297%
17	13.986	1985	1989	1993	rVB	571279	554130	18.27%	2.742%
18	14.086	2001	2006	2012	rBV	369160	376047	12.40%	1.861%
19	14.298	2037	2042	2049	rVB4	20272	34570	1.14%	0.171%
20	14.533	2076	2082	2094	rBV10	22416	74102	2.44%	0.367%
21	14.851	2131	2136	2142	rBV5	23842	38808	1.28%	0.192%
22	15.110	2177	2180	2183	rBV2	38372	39902	1.32%	0.197%
23	15.451	2233	2238	2243	rBV	387105	489806	16.15%	2.424%
24	15.492	2243	2245	2253	rVB	24358	30566	1.01%	0.151%
25	15.927	2314	2319	2324	rBV	49674	71847	2.37%	0.356%
26	16.057	2331	2341	2342	rBV9	42712	85099	2.81%	0.421%
27	17.021	2501	2505	2511	rVB3	21954	38969	1.28%	0.193%

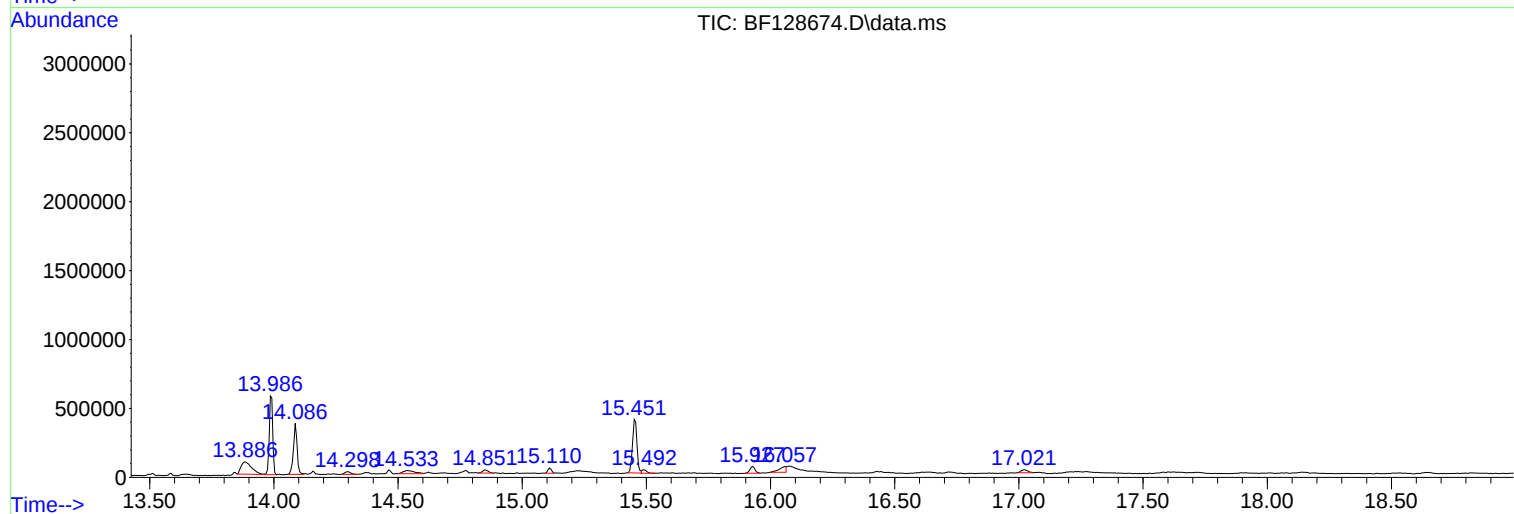
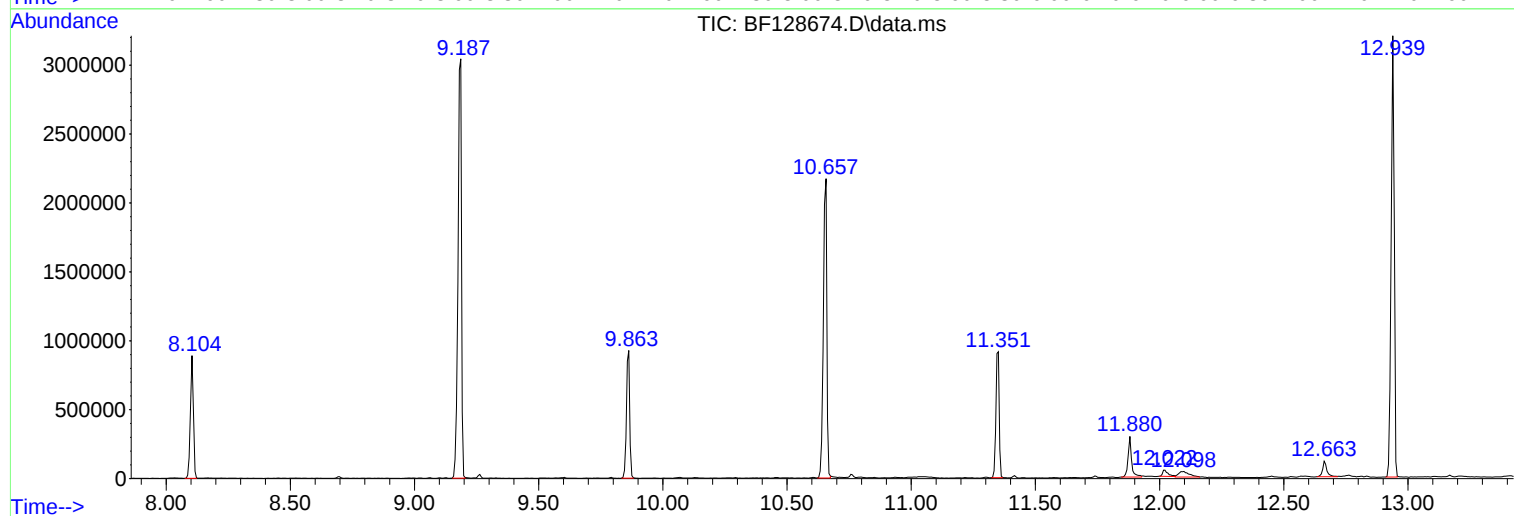
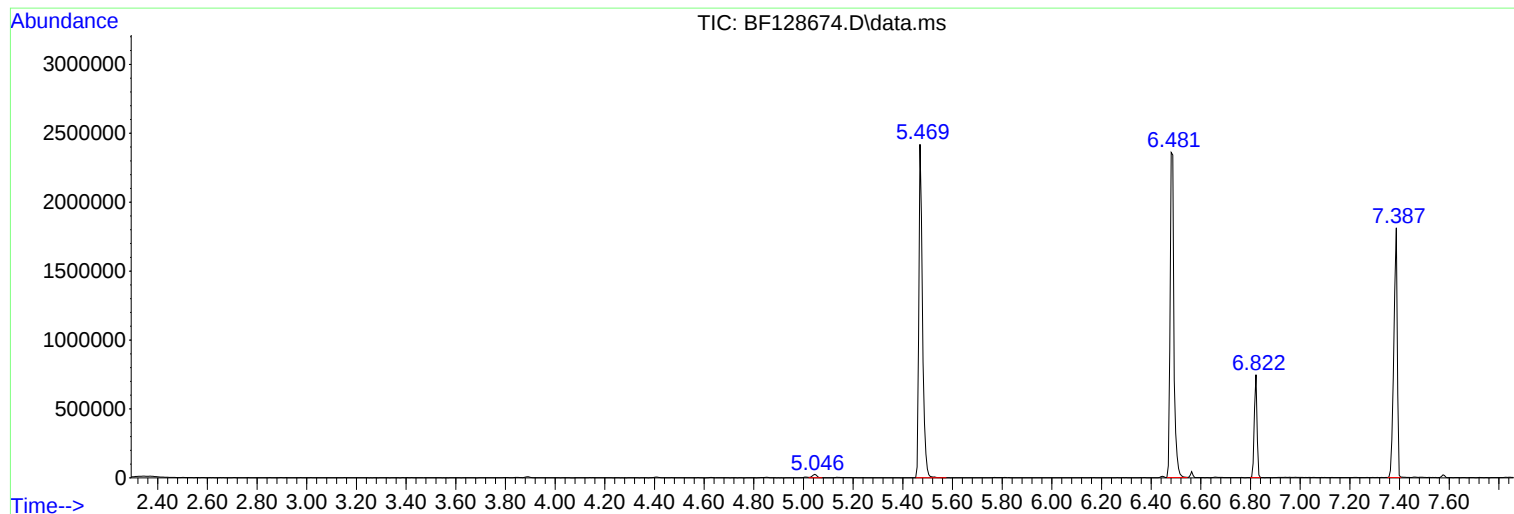
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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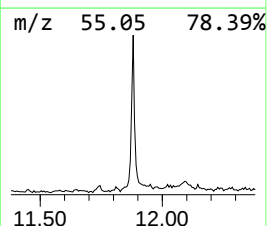
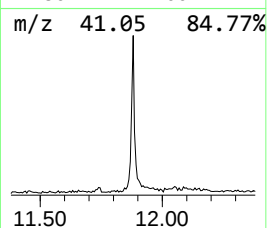
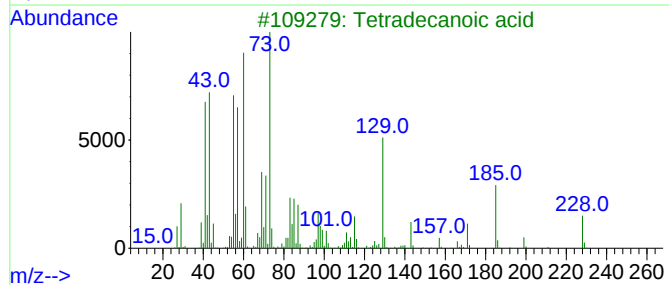
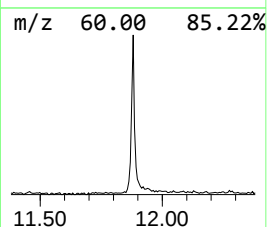
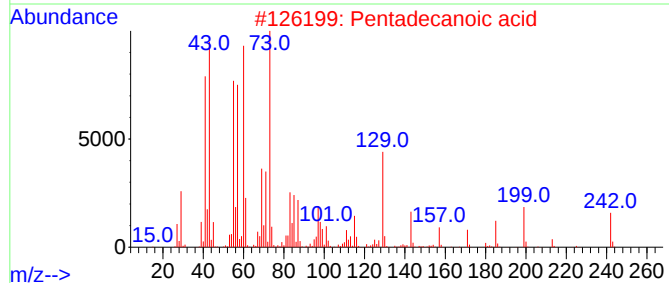
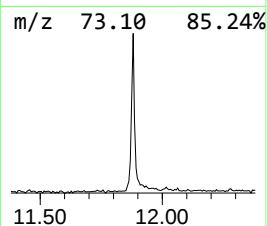
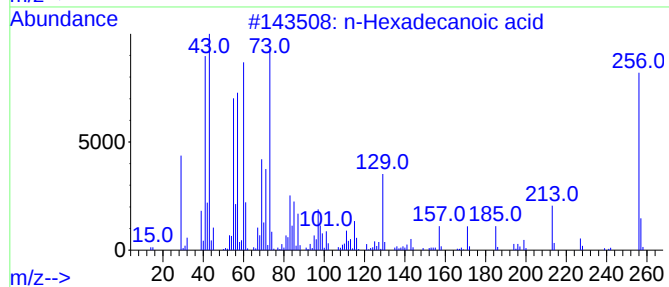
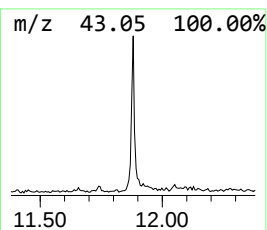
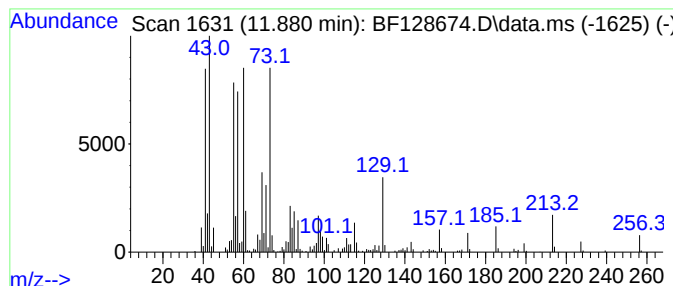
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.881	6.82 ng	290243	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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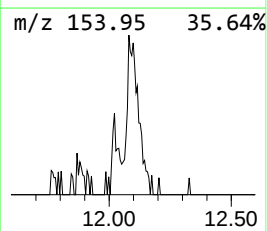
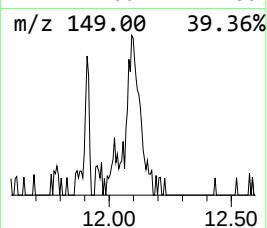
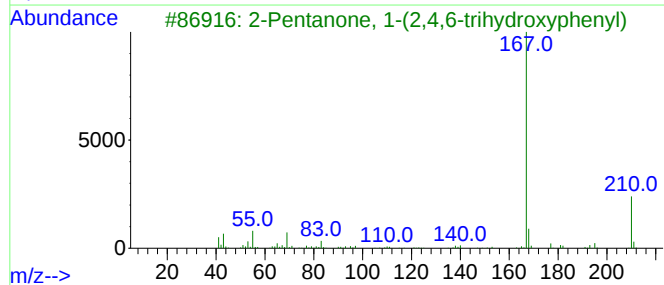
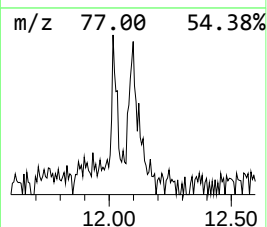
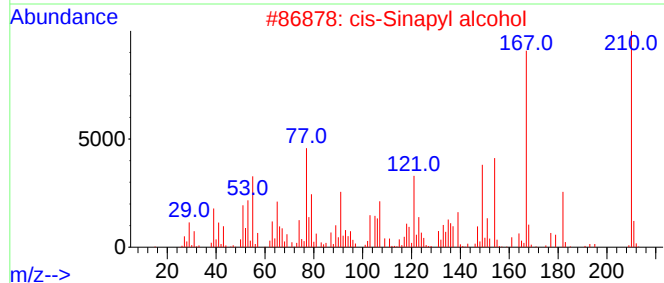
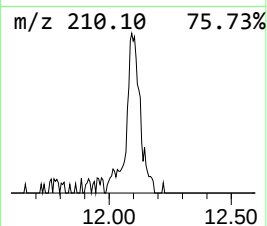
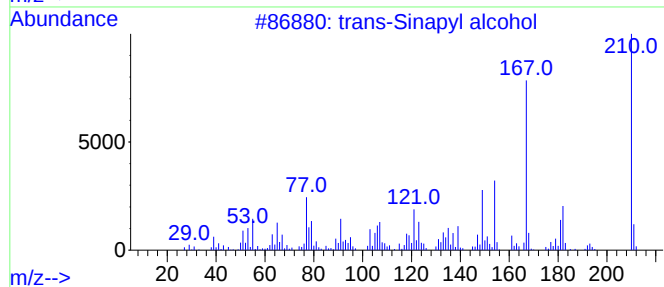
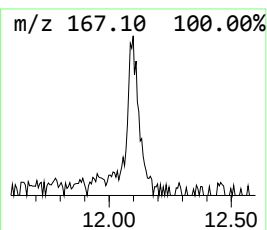
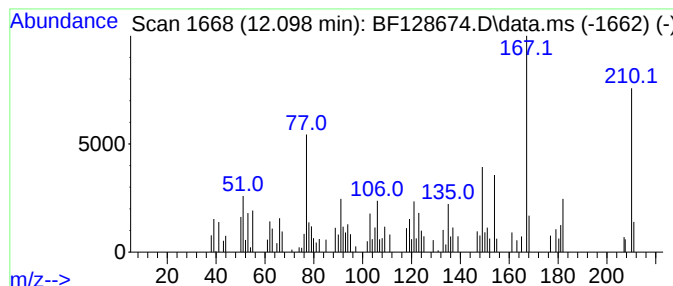
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 trans-Sinapyl alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	2.78 ng	118345	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	90
2			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	89
3			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	38
4			2-(1,3-Benzoxazol-2-yl)aniline	210	C13H10N2O	029483-74-7	30
5			3H-Indazol-3-one, 1,2-dihydro-1-...	210	C13H10N2O	028561-80-0	30



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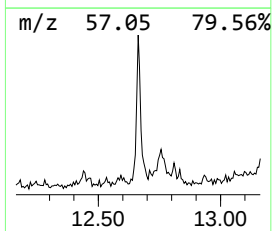
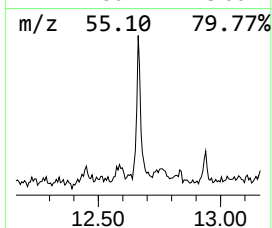
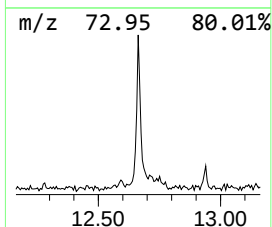
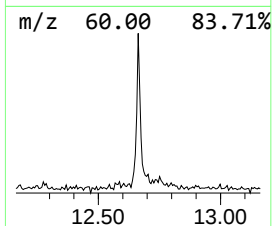
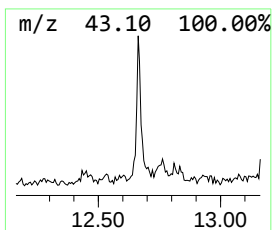
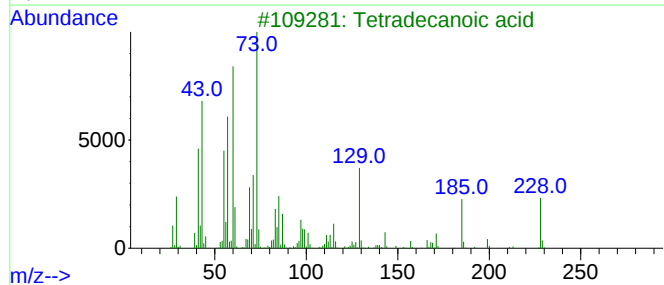
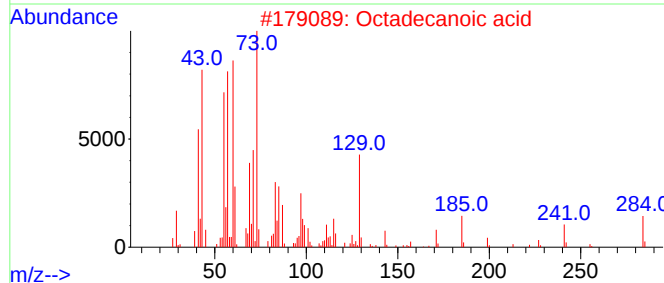
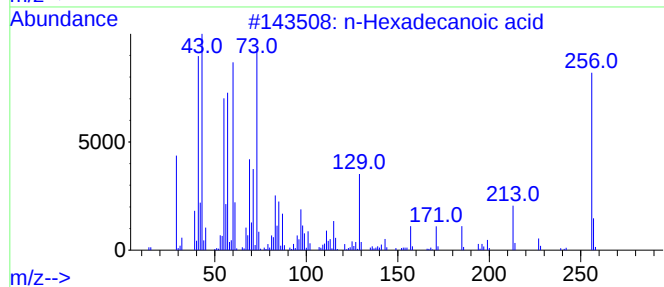
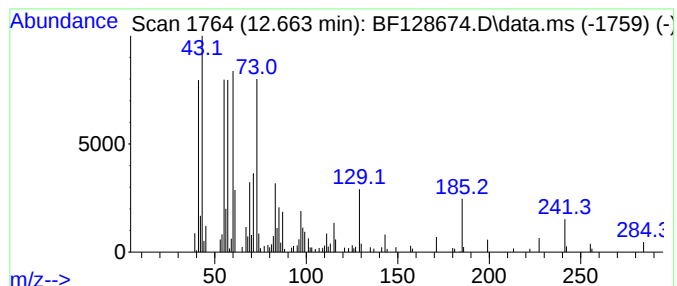
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	3.21 ng	136643	Phenanthrene-d10	11.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Octadecanoic acid	284	C18H36O2	000057-11-4	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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ALS Vial : 6 Sample Multiplier: 1

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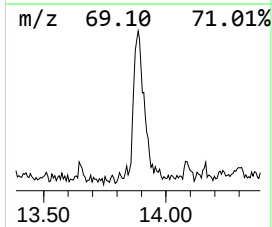
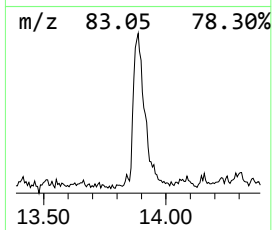
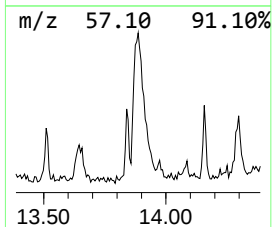
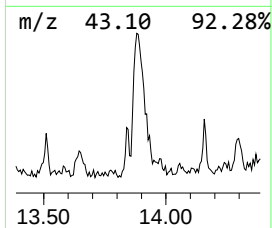
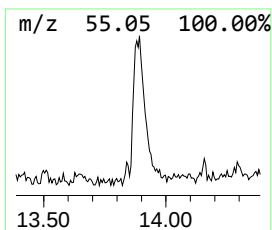
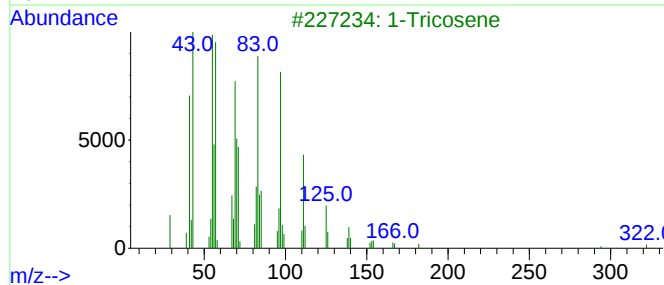
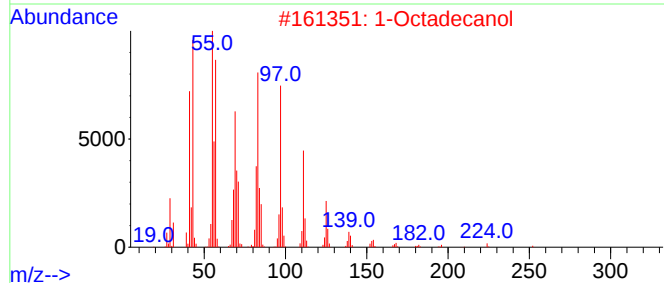
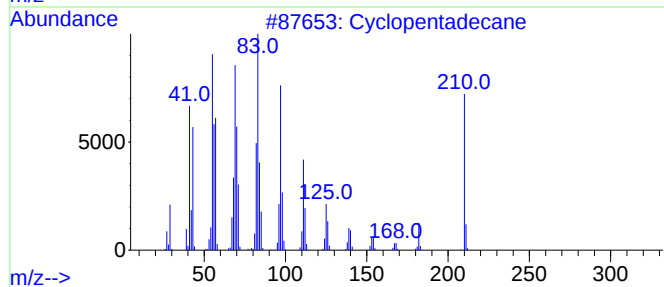
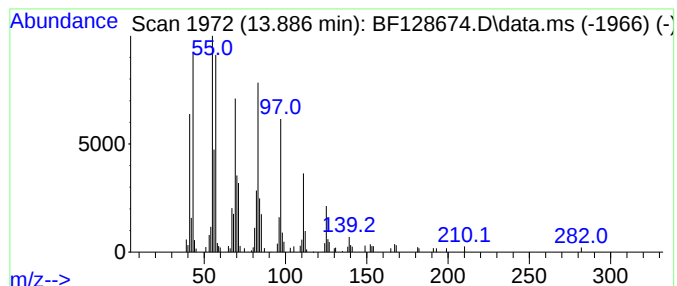
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	9.46 ng	262101	Chrysene-d12	13.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	91
2		1-Octadecanol	270	C18H38O	000112-92-5	91
3		1-Tricosene	322	C23H46	018835-32-0	90
4		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	90
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	90



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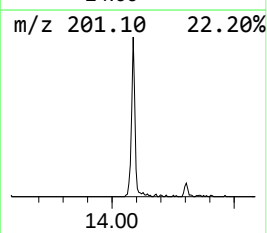
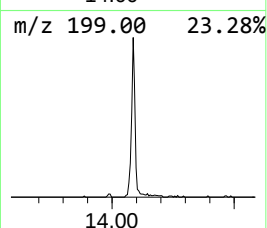
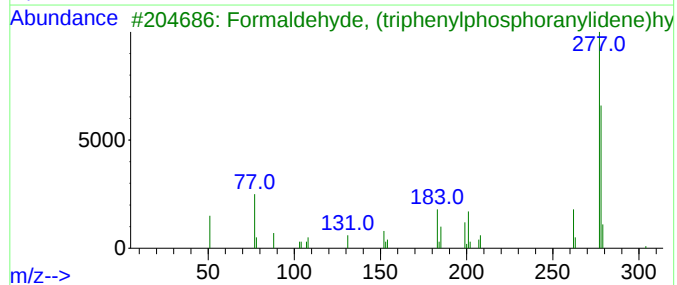
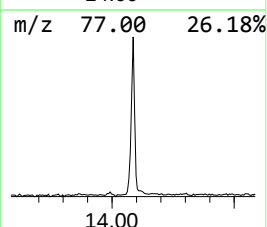
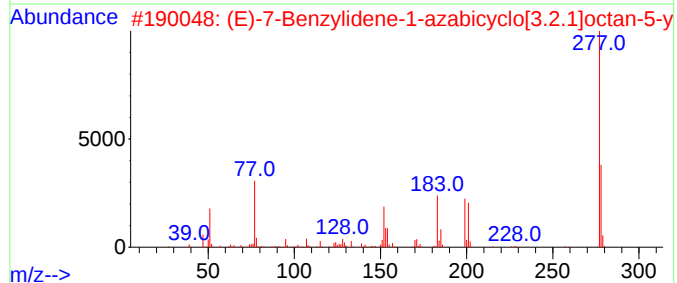
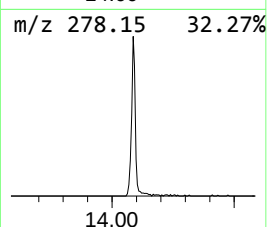
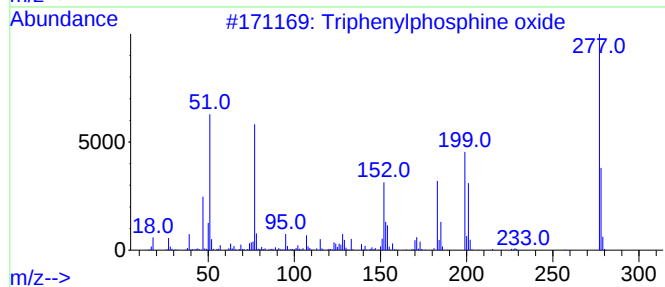
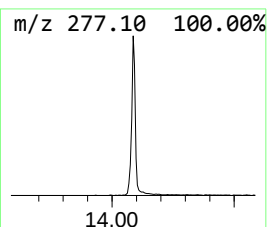
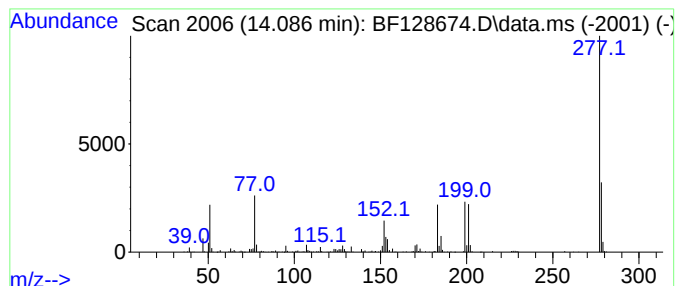
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	13.57 ng	376047	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-ylidene triphenylphosphine oxide	293	C15H19NO3S	1000483-83-4	81
3			Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38
5			Carbazol-1-one, 1,2,3,4-tetrahyd	277	C18H15NO2	299962-12-2	23



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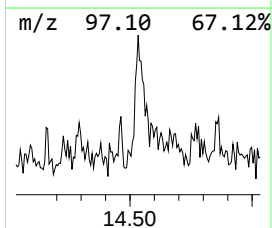
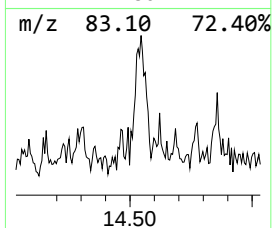
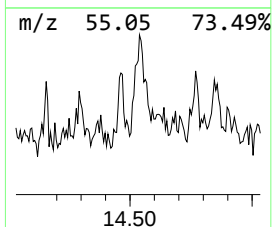
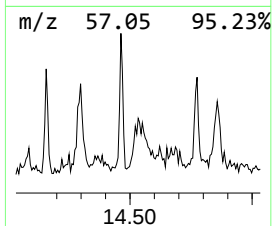
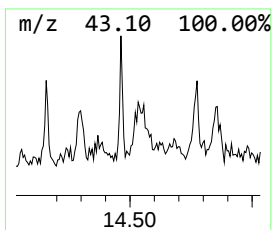
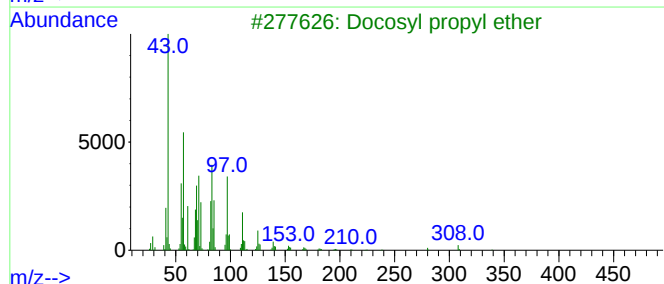
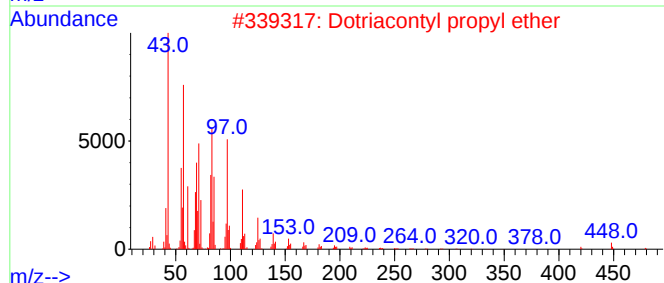
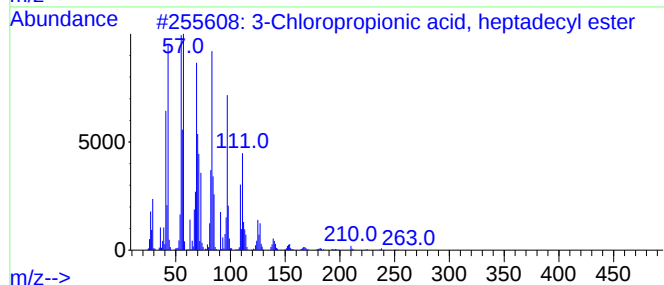
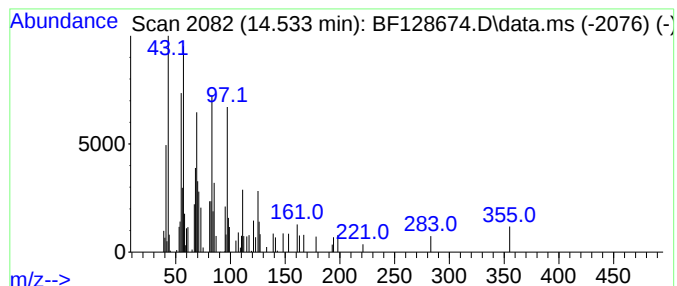
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.67 ng	74102	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	60
2			Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	58
3			Docosyl propyl ether	368	C25H52O	1000406-28-2	58
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	53
5			17-Pentatriacontene	491	C35H70	006971-40-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128674.D
Acq On : 03 Jun 2022 12:17
Operator : CG\JU
Sample : N2987-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P027-SS004-0006-01

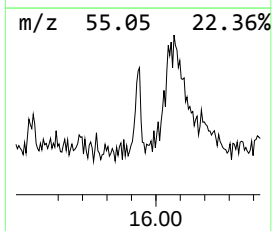
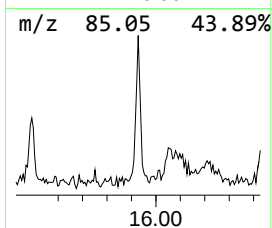
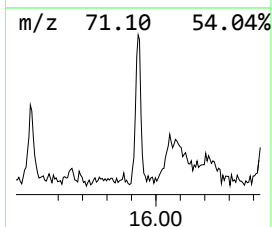
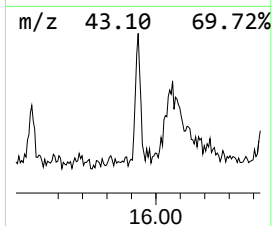
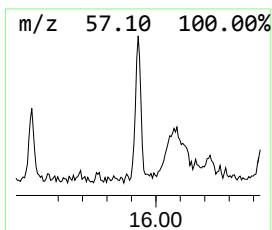
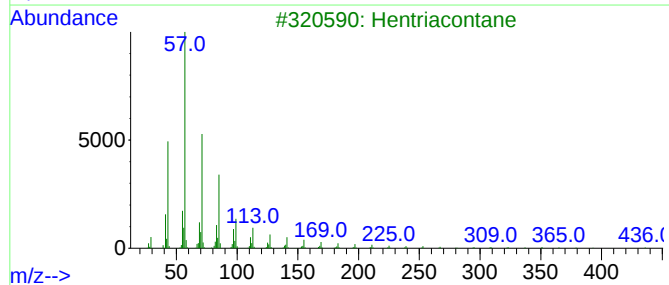
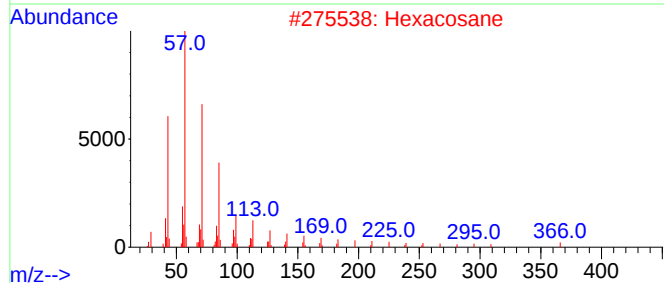
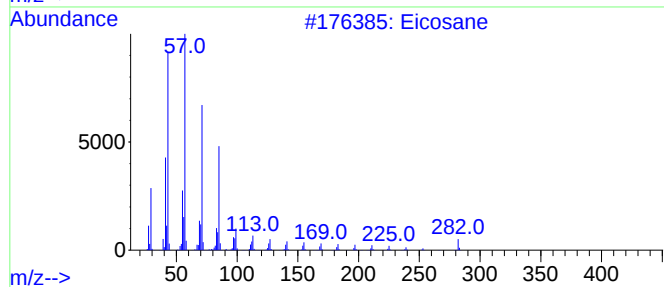
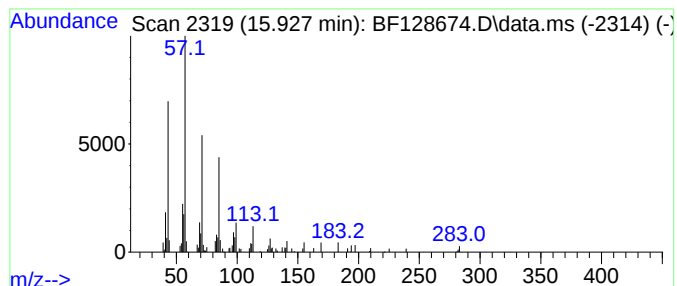
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	2.93 ng	71847	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Hexacosane	366	C26H54	000630-01-3	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128674.D
Acq On : 03 Jun 2022 12:17
Operator : CG\JU
Sample : N2987-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P027-SS004-0006-01

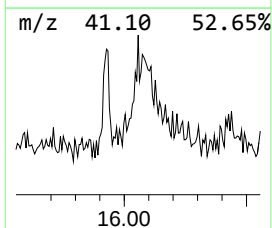
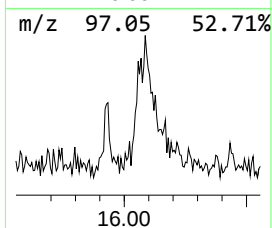
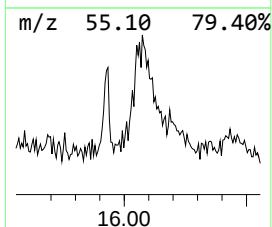
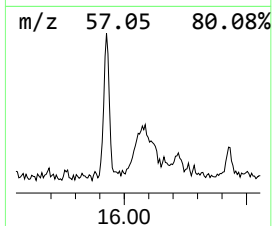
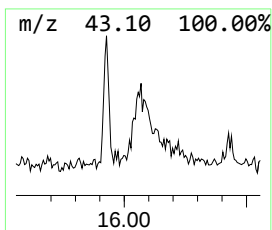
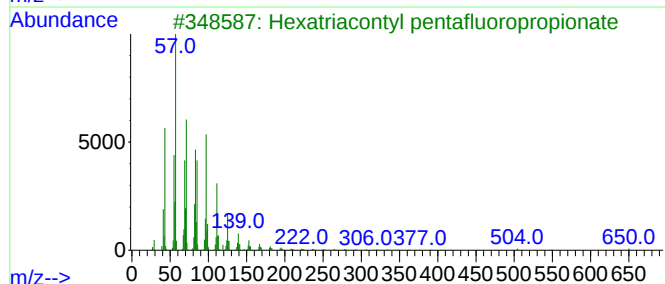
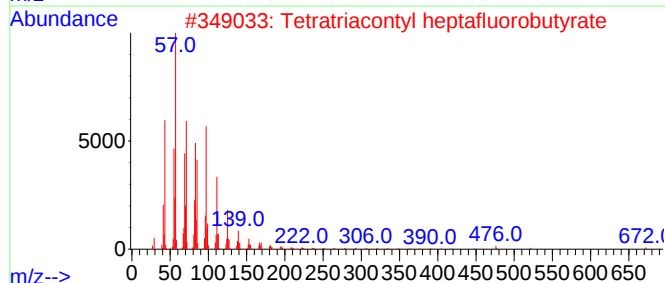
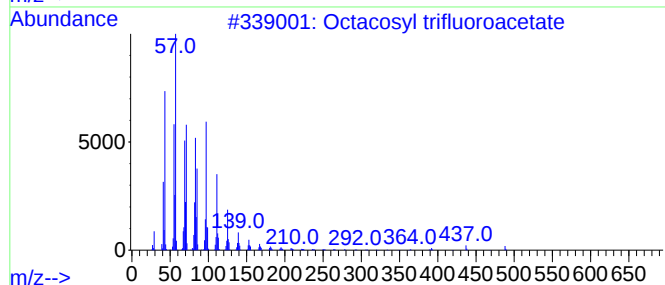
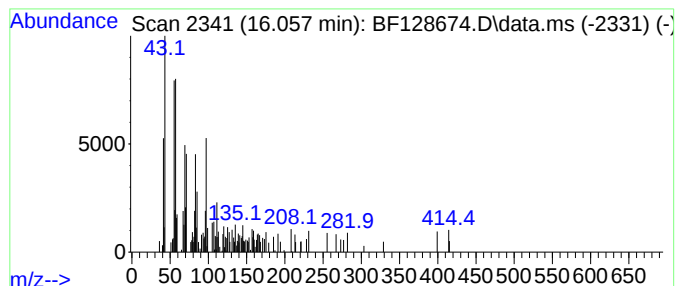
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	3.47 ng	85099	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81
2			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	81
3			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	81
4			Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	81
5			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128674.D
Acq On : 03 Jun 2022 12:17
Operator : CG\JU
Sample : N2987-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P027-SS004-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
n-Hexadecanoic ...	11.881	6.8	ng	290243	4	11.351	850615	20.0
trans-Sinapyl a...	12.098	2.8	ng	118345	4	11.351	850615	20.0
Octadecanoic acid	12.663	3.2	ng	136643	4	11.351	850615	20.0
Cyclopentadecane	13.886	9.5	ng	262101	5	13.992	554130	20.0
Triphenylphosph...	14.086	13.6	ng	376047	5	13.992	554130	20.0
3-Chloropropion...	14.533	2.7	ng	74102	5	13.992	554130	20.0
Eicosane	15.927	2.9	ng	71847	6	15.451	489806	20.0
Octacosyl trifl...	16.057	3.5	ng	85099	6	15.451	489806	20.0