

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
 Data File : BF128462.D
 Acq On : 25 May 2022 16:25
 Operator : CG\JU
 Sample : N2896-20
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P040-SS001-1824-01

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-BF052022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	465	468	478	rBV	15547	23195	1.21%	0.164%
2	5.434	531	535	556	rBV	1837204	1801139	94.10%	12.751%
3	6.451	704	708	723	rBV	1828133	1794206	93.74%	12.702%
4	6.557	723	726	732	rVB	23150	27073	1.41%	0.192%
5	6.804	765	768	775	rBV	578108	539759	28.20%	3.821%
6	7.375	861	865	874	rBV	1286064	1181866	61.75%	8.367%
7	8.092	983	987	990	rBV	671332	636295	33.24%	4.504%
8	9.163	1164	1169	1173	rBV	2036955	1913983	100.00%	13.549%
9	9.275	1184	1188	1191	rBV2	25551	26261	1.37%	0.186%
10	9.433	1211	1215	1217	rBV	31350	24675	1.29%	0.175%
11	9.845	1281	1285	1289	rVB	798508	643446	33.62%	4.555%
12	10.639	1416	1420	1429	rBV	1139724	1038783	54.27%	7.354%
13	10.739	1434	1437	1446	rVB6	9765	20301	1.06%	0.144%
14	11.339	1535	1539	1542	rBV	747717	616689	32.22%	4.366%
15	11.586	1574	1581	1588	rBV8	28317	71854	3.75%	0.509%
16	11.716	1600	1603	1606	rBV	110991	94156	4.92%	0.667%
17	11.863	1624	1628	1641	rBV2	83189	113482	5.93%	0.803%
18	12.427	1721	1724	1733	rVB	258277	271614	14.19%	1.923%
19	12.510	1735	1738	1743	rVB	111795	94102	4.92%	0.666%
20	12.569	1743	1748	1751	rBV	123636	112541	5.88%	0.797%
21	12.645	1759	1761	1766	rBV3	17664	22590	1.18%	0.160%
22	12.816	1786	1790	1796	rBV	54829	85038	4.44%	0.602%
23	12.921	1804	1808	1812	rBV	1754681	1681129	87.83%	11.901%
24	13.392	1886	1888	1894	rVB2	25314	24527	1.28%	0.174%
25	13.480	1900	1903	1907	rBV2	18493	20121	1.05%	0.142%
26	13.845	1961	1965	1974	rBV3	61579	120925	6.32%	0.856%
27	13.951	1980	1983	1985	rVB	51518	43120	2.25%	0.305%
28	13.986	1986	1989	1993	rBV	586823	536195	28.01%	3.796%
29	14.080	2002	2005	2008	rBV	48327	46976	2.45%	0.333%
30	14.127	2011	2013	2019	rVV3	22918	22558	1.18%	0.160%
31	14.433	2063	2065	2069	rVB	30396	29185	1.52%	0.207%
32	15.457	2235	2239	2247	rVB2	352868	448143	23.41%	3.172%

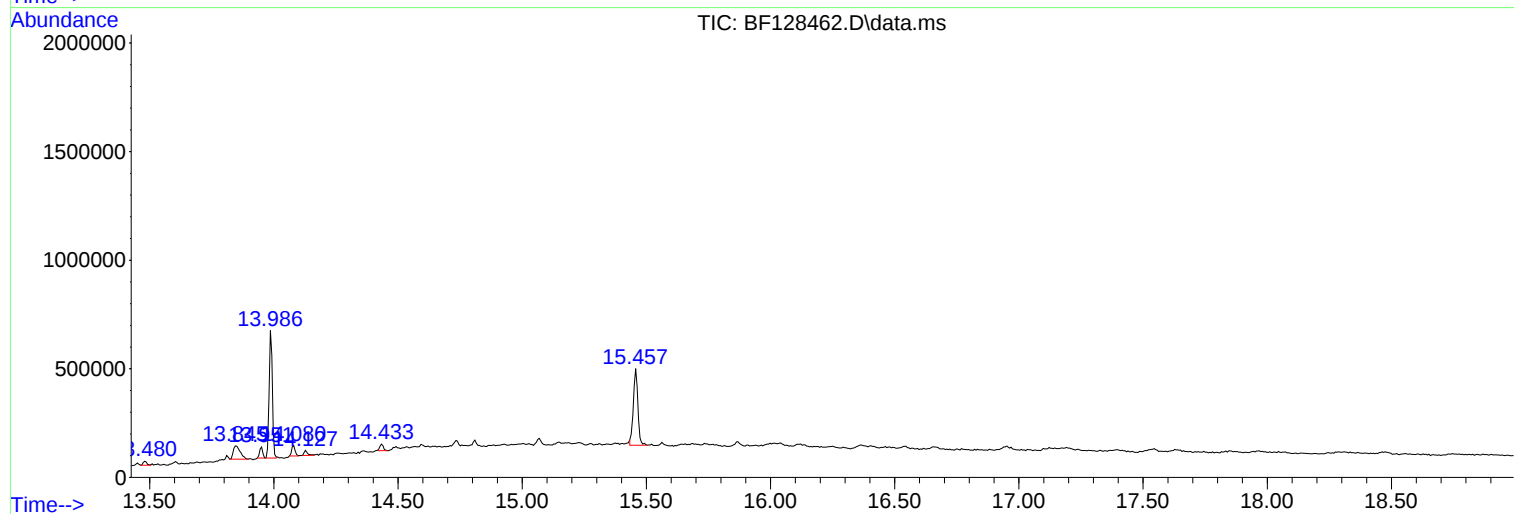
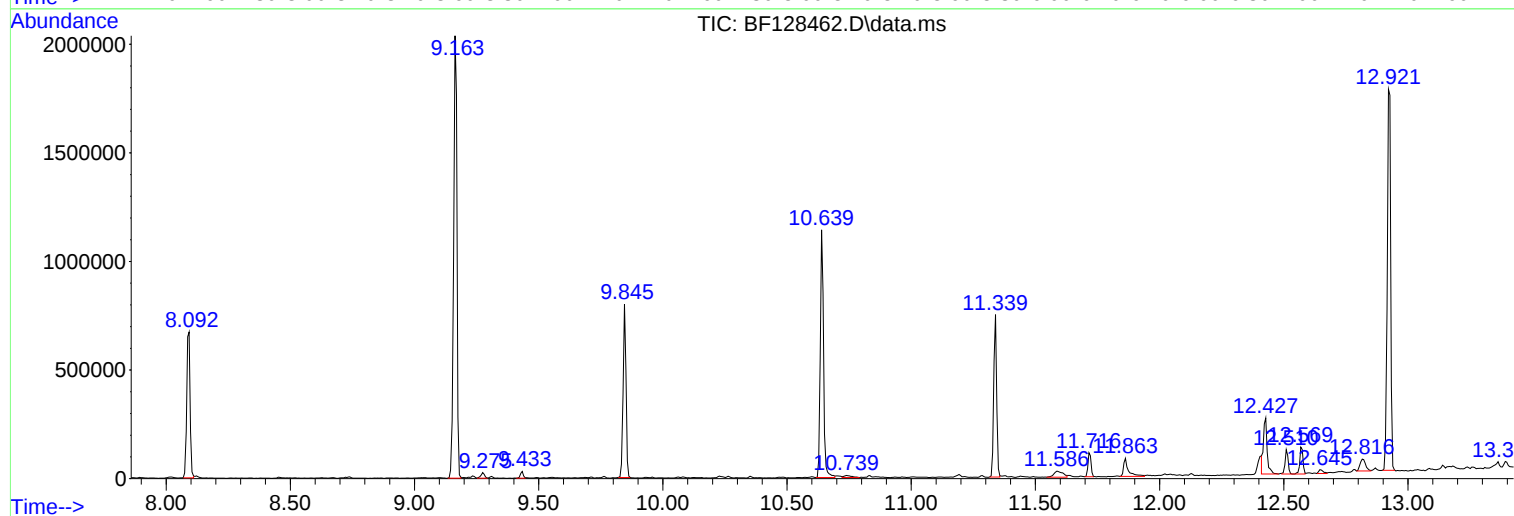
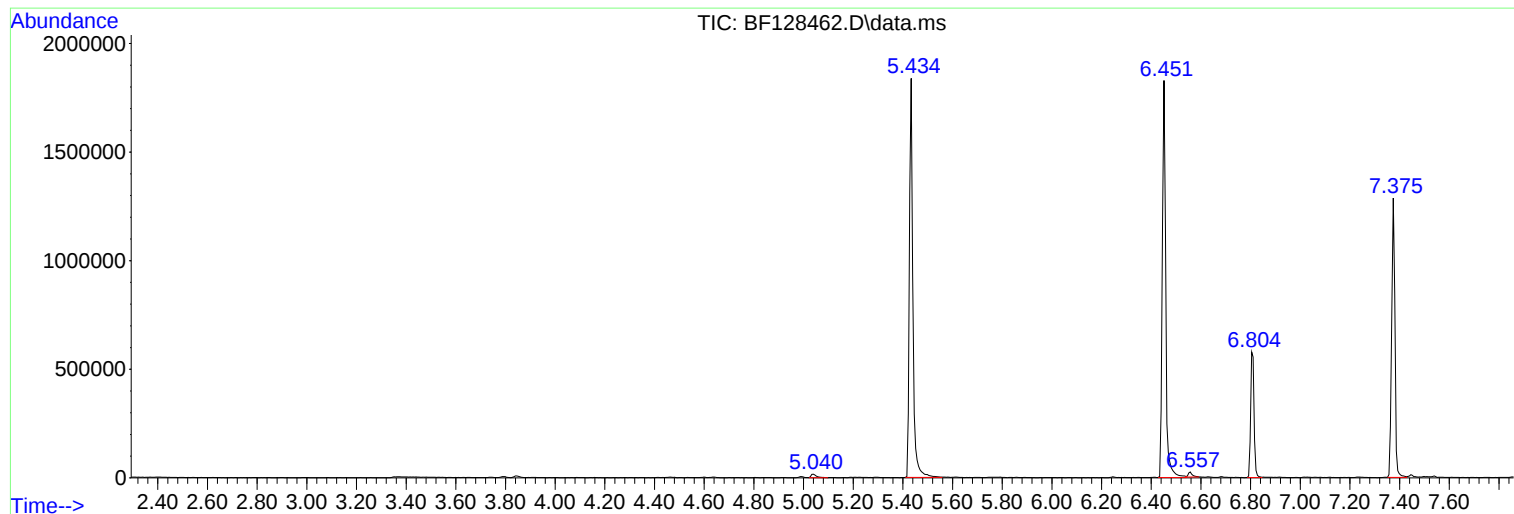
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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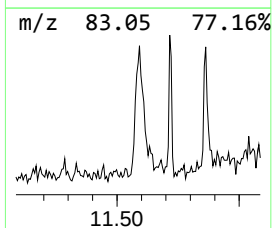
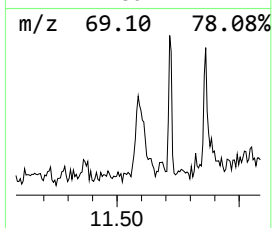
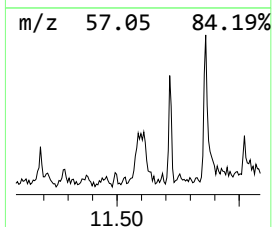
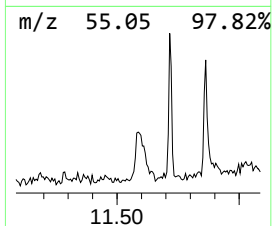
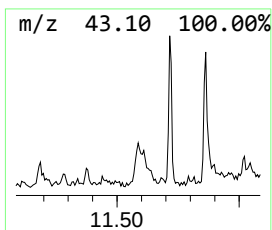
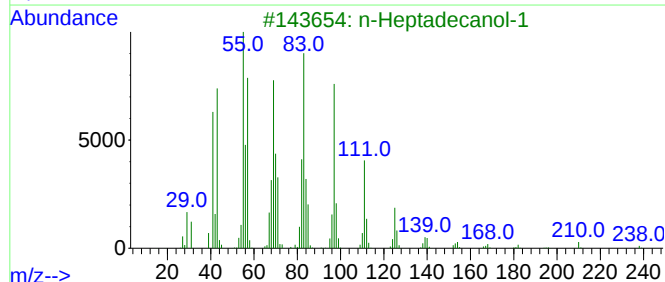
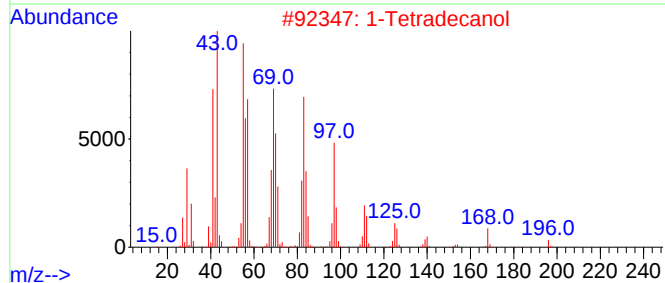
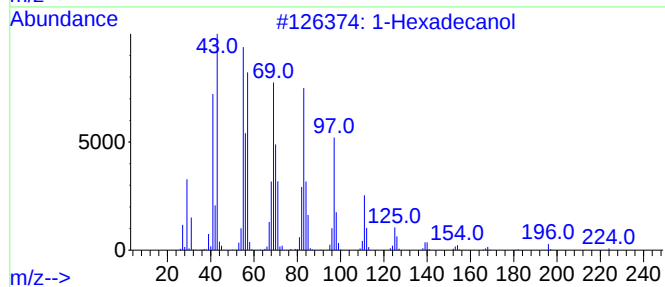
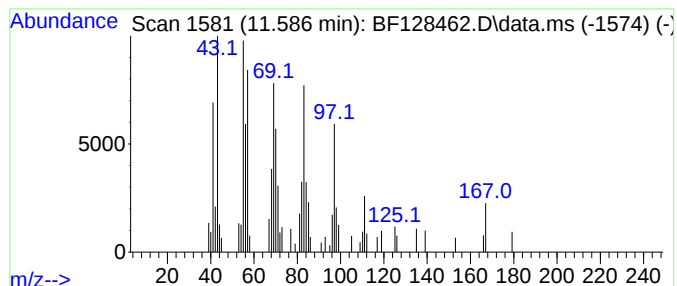
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.586	2.33 ng	71854	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol			242	C16H34O	036653-82-4	93
2	1-Tetradecanol			214	C14H30O	000112-72-1	90
3	n-Heptadecanol-1			256	C17H36O	001454-85-9	90
4	4-Heptafluorobutyryloxyhexadecane			438	C20H33F7O2	1010282-97-2	87
5	5-Octadecene, (E)-			252	C18H36	007206-21-5	83



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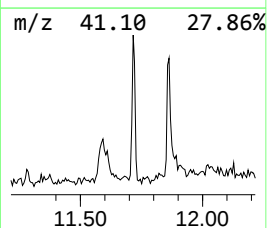
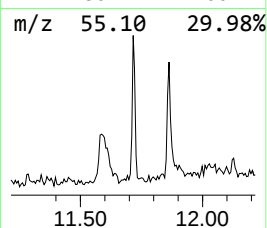
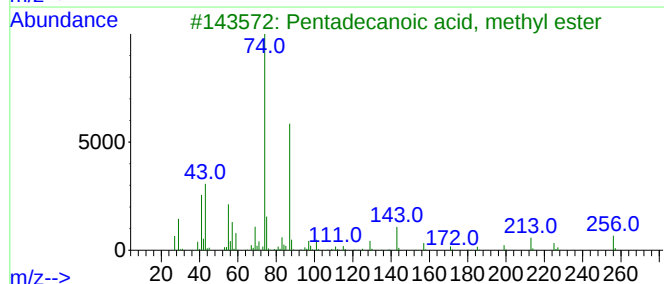
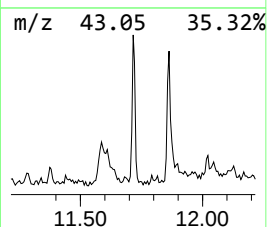
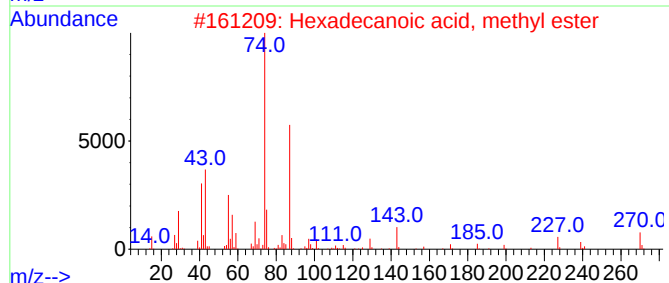
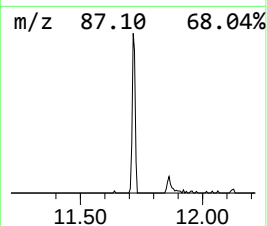
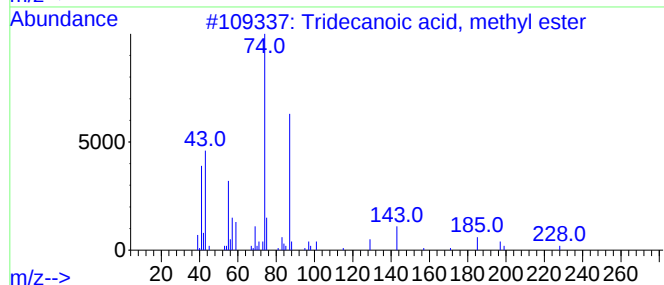
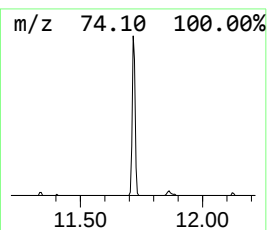
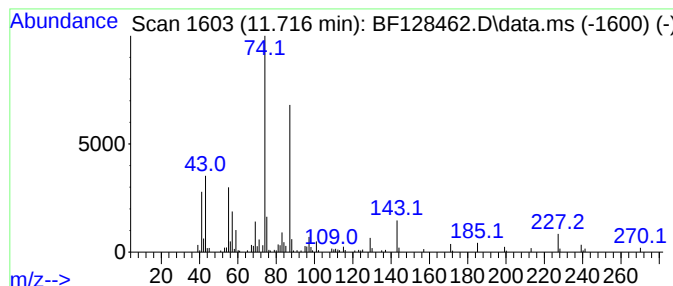
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tridecanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	3.05 ng	94156	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86



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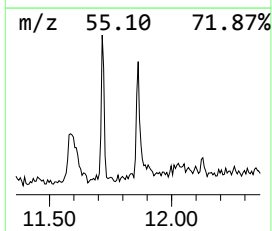
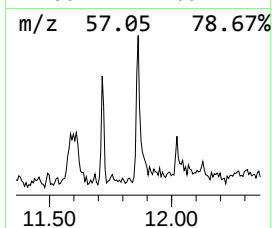
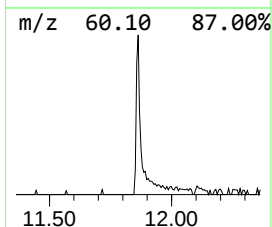
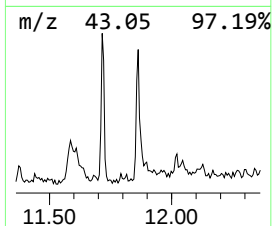
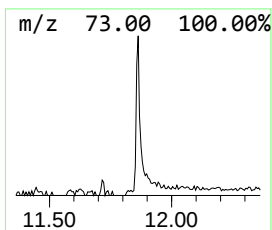
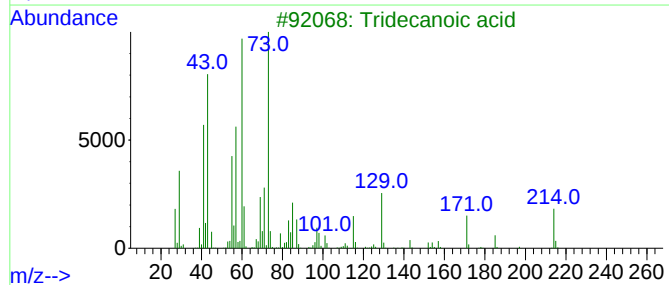
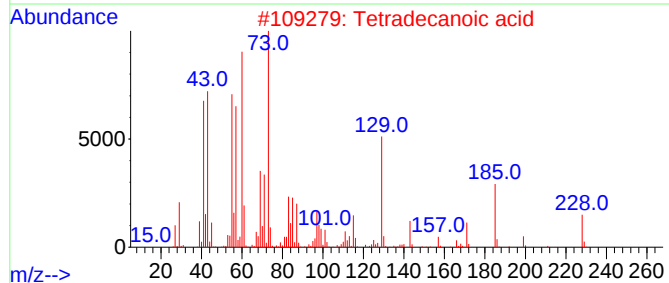
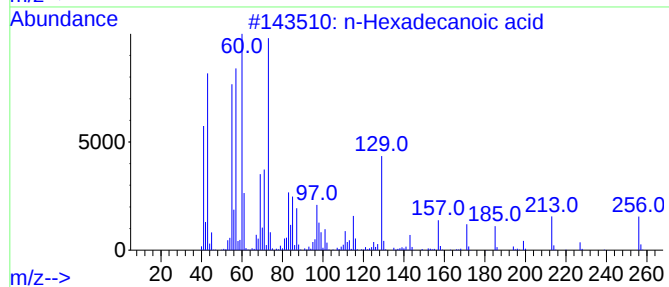
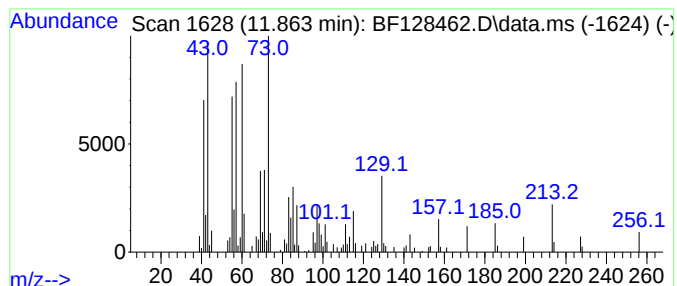
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.68 ng	113482	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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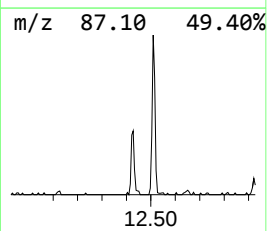
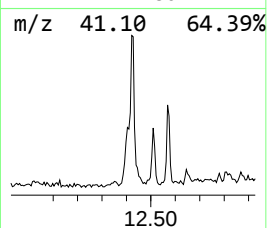
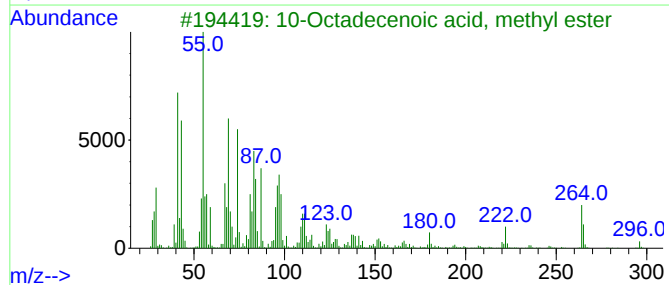
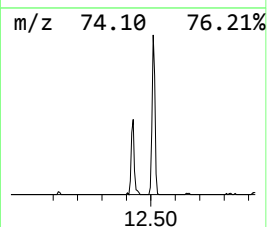
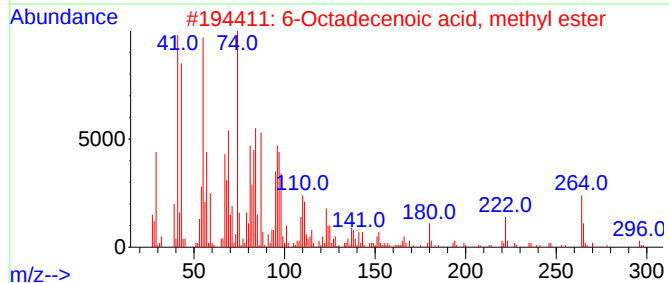
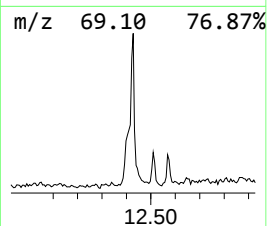
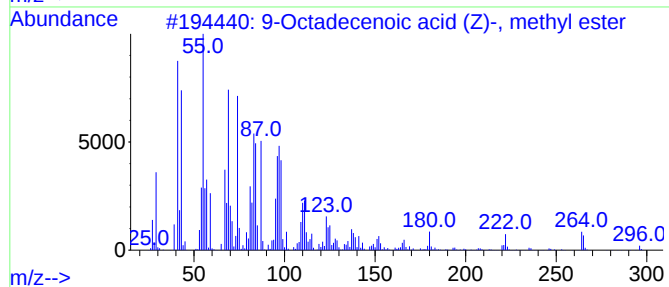
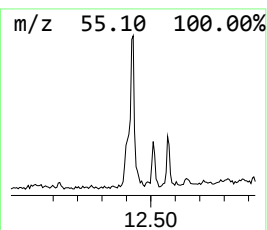
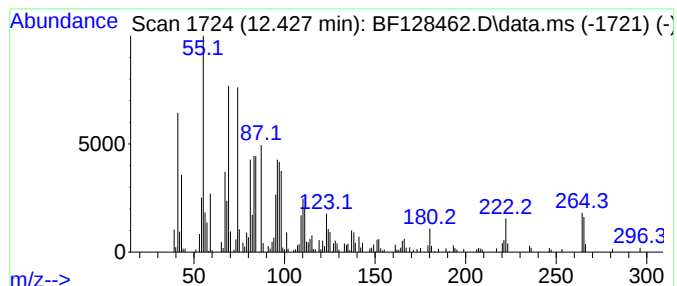
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	8.81 ng	271614	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



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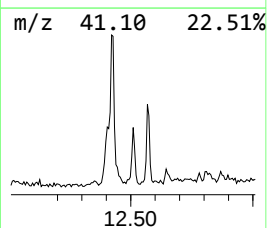
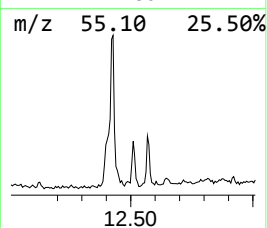
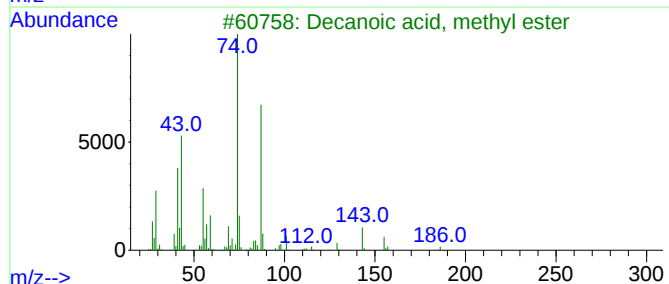
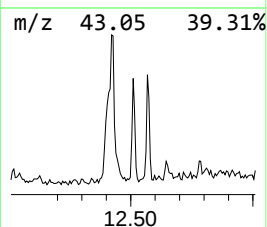
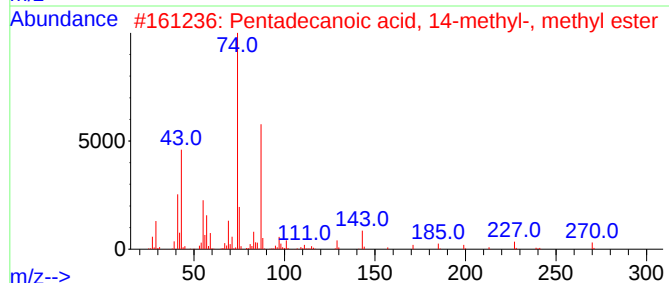
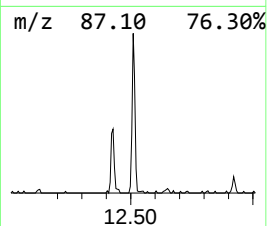
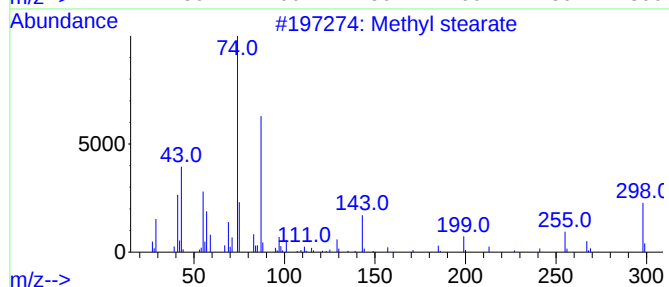
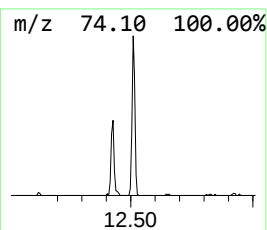
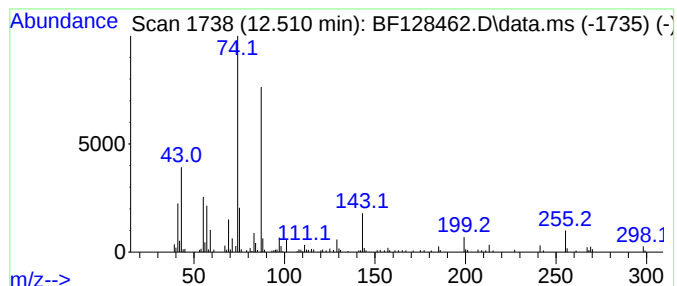
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	3.05 ng	94102	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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P040-SS001-1824-01

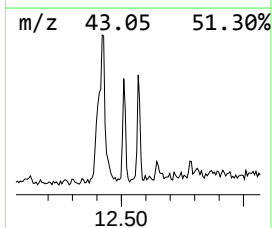
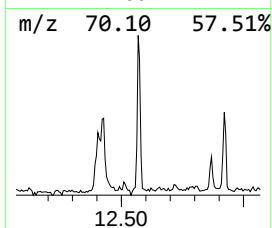
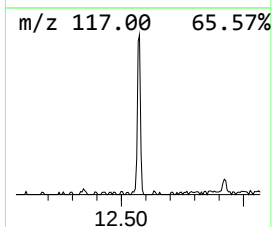
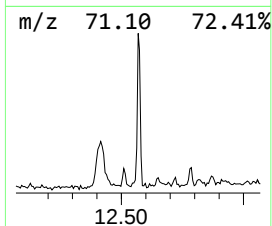
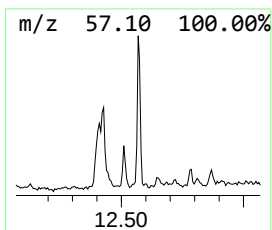
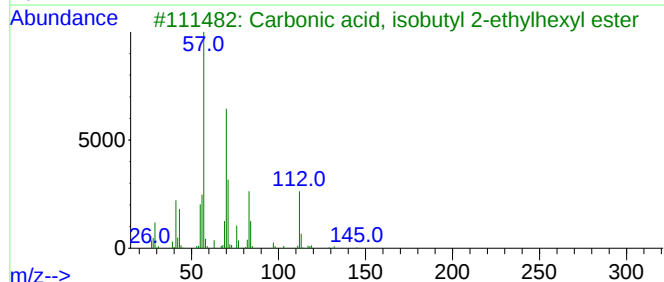
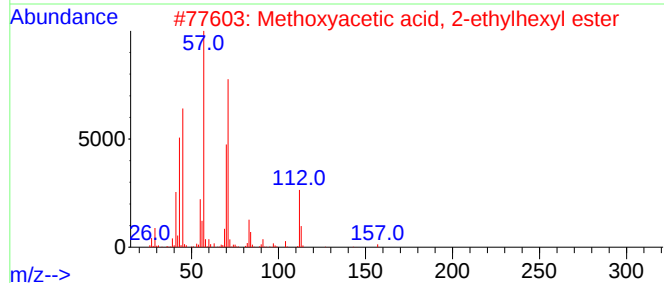
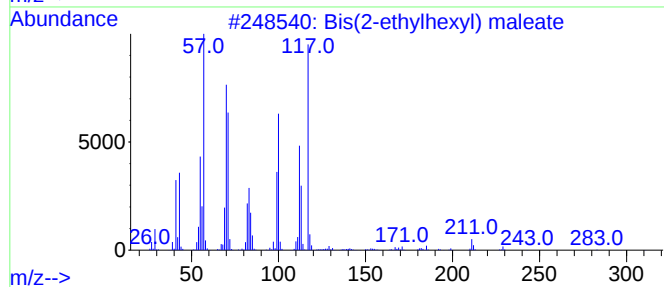
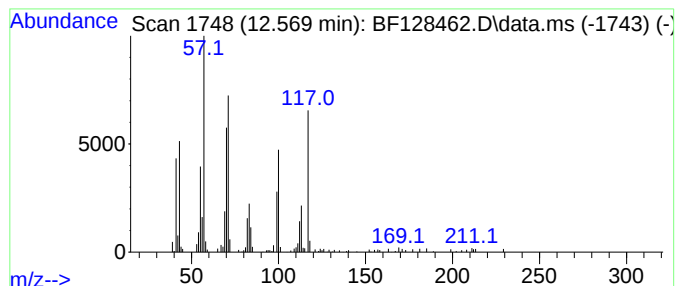
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	3.65 ng	112541	Phenanthrene-d10	11.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	91
2			Methoxyacetic acid, 2-ethylhexyl...	202	C11H22O3	1000282-41-4	35
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	35
4			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	35
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128462.D
Acq On : 25 May 2022 16:25
Operator : CG\JU
Sample : N2896-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P040-SS001-1824-01

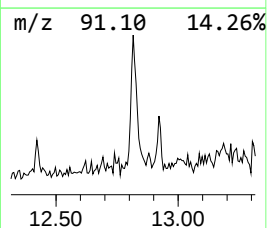
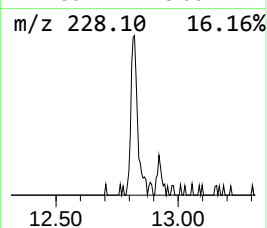
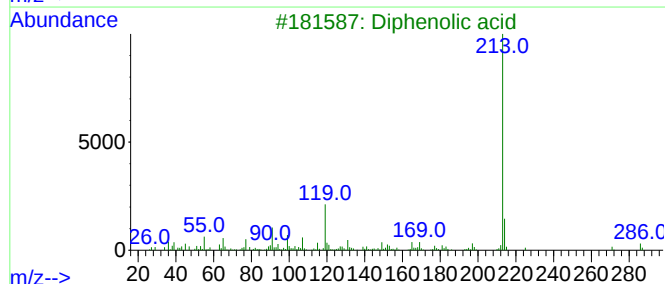
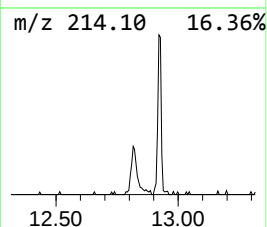
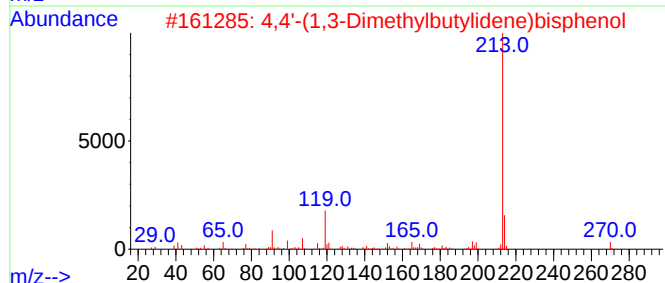
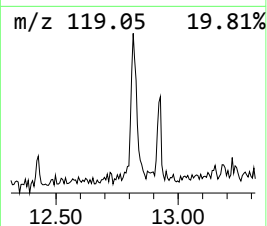
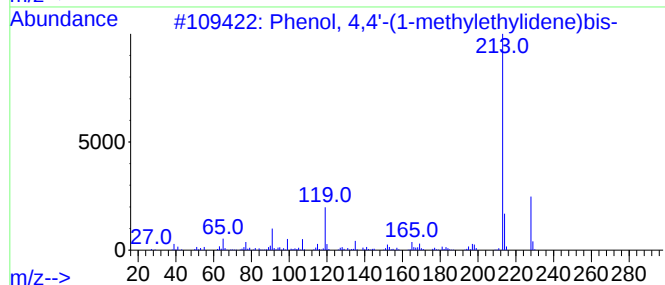
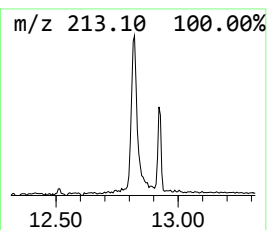
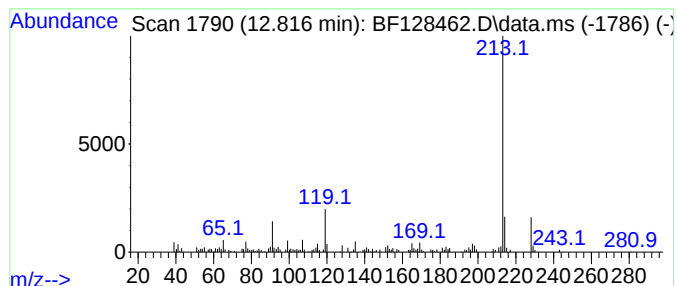
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	3.17 ng	85038	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	83
3			Diphenolic acid	286	C17H18O4	000126-00-1	80
4			2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	80
5			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128462.D
Acq On : 25 May 2022 16:25
Operator : CG\JU
Sample : N2896-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P040-SS001-1824-01

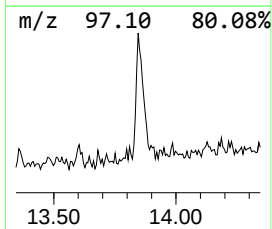
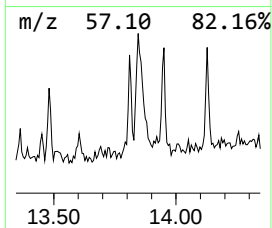
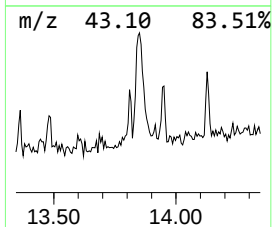
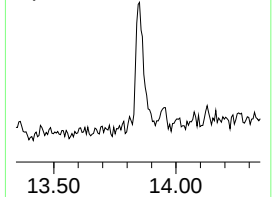
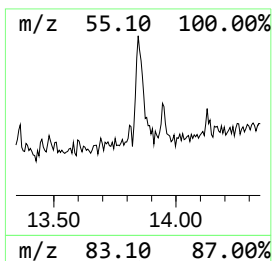
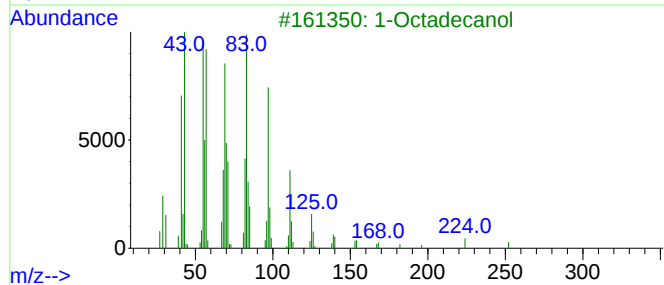
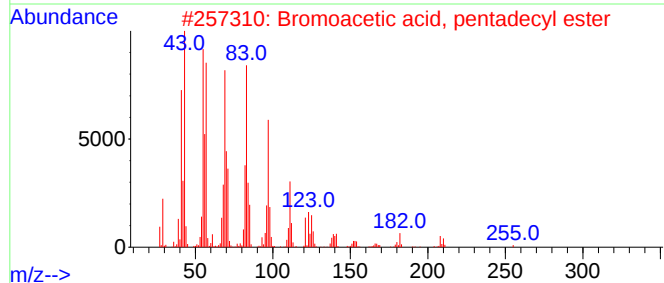
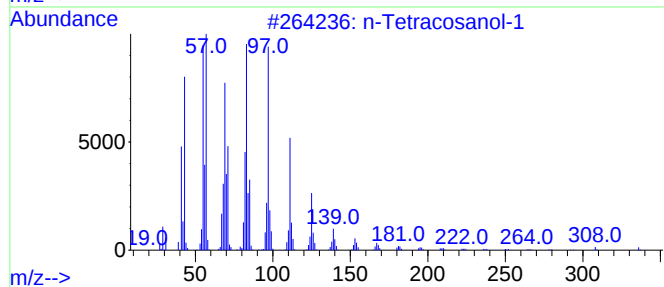
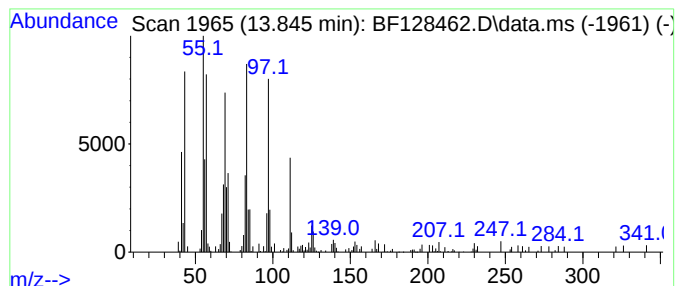
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	4.51 ng	120925	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	80
2			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	68
3			1-Octadecanol	270	C18H38O	000112-92-5	68
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	58
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128462.D
Acq On : 25 May 2022 16:25
Operator : CG\JU
Sample : N2896-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P040-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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
1-Hexadecanol	11.586	2.3	ng	71854	4	11.339	616689	20.0
Tridecanoic aci...	11.716	3.0	ng	94156	4	11.339	616689	20.0
n-Hexadecanoic ...	11.863	3.7	ng	113482	4	11.339	616689	20.0
9-Octadecenoic ...	12.427	8.8	ng	271614	4	11.339	616689	20.0
Methyl stearate	12.510	3.0	ng	94102	4	11.339	616689	20.0
Bis(2-ethylhexy...	12.569	3.6	ng	112541	4	11.339	616689	20.0
Phenol, 4,4'-(1...	12.816	3.2	ng	85038	5	13.986	536195	20.0
n-Tetracosanol-1	13.845	4.5	ng	120925	5	13.986	536195	20.0