

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111920\
 Data File : BF122379.D
 Acq On : 19 Nov 2020 14:29
 Operator : JU/CG
 Sample : L4797-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-LA-2-5-WC

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-BF110920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	42	rVB	487343	952933	17.58%	1.945%
2	5.475	571	576	579	rBV	4263585	3873683	71.45%	7.905%
3	6.481	742	747	766	rBV	3959655	4234278	78.10%	8.641%
4	6.863	809	812	815	rBV	1811852	1407232	25.96%	2.872%
5	7.422	902	907	910	rBV	2919546	2579434	47.58%	5.264%
6	8.145	1026	1030	1034	rBV	2042833	1882210	34.72%	3.841%
7	9.222	1209	1213	1217	rBV	4719445	4539303	83.72%	9.264%
8	9.339	1231	1233	1238	rVB	82147	81353	1.50%	0.166%
9	9.616	1276	1280	1284	rBV	258838	220310	4.06%	0.450%
10	9.904	1325	1329	1338	rVB	2681779	2284466	42.13%	4.662%
11	10.686	1458	1462	1478	rBV	2658398	2650503	48.89%	5.409%
12	11.386	1577	1581	1585	rBV	2745494	2386963	44.03%	4.871%
13	11.921	1663	1672	1694	rBV	1820351	3037455	56.02%	6.199%
14	12.186	1714	1717	1724	rVB	163701	158609	2.93%	0.324%
15	12.574	1779	1783	1786	rBV	106899	136664	2.52%	0.279%
16	12.710	1788	1806	1818	rVV	2328483	4486081	82.74%	9.155%
17	12.874	1832	1834	1841	rVB5	56142	61630	1.14%	0.126%
18	12.974	1847	1851	1854	rBV	6068468	5421781	100.00%	11.065%
19	13.210	1888	1891	1896	rBV2	60431	69814	1.29%	0.142%
20	13.886	2002	2006	2014	rBV3	334808	671724	12.39%	1.371%
21	13.962	2016	2019	2025	rVB3	136516	244393	4.51%	0.499%
22	14.027	2026	2030	2033	rVV	2829177	2485185	45.84%	5.072%
23	14.198	2056	2059	2062	rBV	99400	83086	1.53%	0.170%
24	14.504	2108	2111	2114	rVB	175512	161253	2.97%	0.329%
25	14.809	2161	2163	2170	rVB2	114210	115948	2.14%	0.237%
26	14.904	2176	2179	2182	rVB3	131762	138630	2.56%	0.283%
27	15.115	2209	2215	2219	rBV4	209780	502692	9.27%	1.026%
28	15.151	2219	2221	2229	rVB2	184715	231473	4.27%	0.472%
29	15.498	2274	2280	2284	rBV	1848910	2432151	44.86%	4.964%
30	15.974	2359	2361	2367	rVB2	76227	97536	1.80%	0.199%
31	16.333	2417	2422	2433	rVB6	158708	467273	8.62%	0.954%
32	18.533	2789	2796	2803	rBV3	91319	279115	5.15%	0.570%
33	18.874	2847	2854	2870	rVB5	171880	625115	11.53%	1.276%

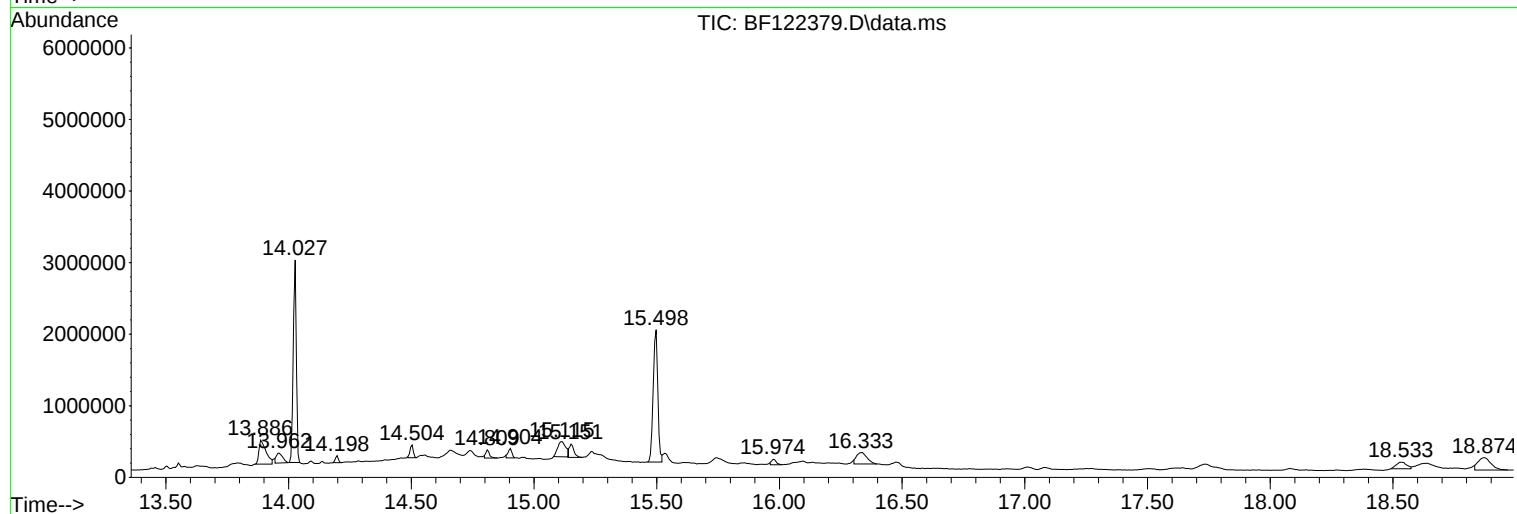
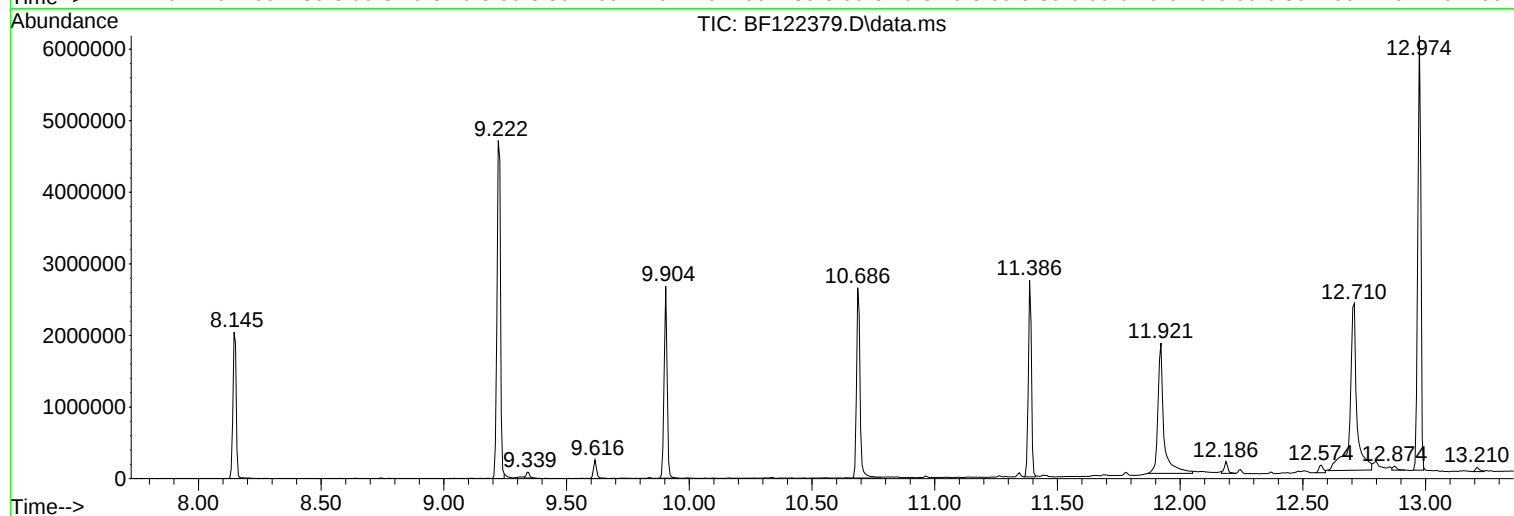
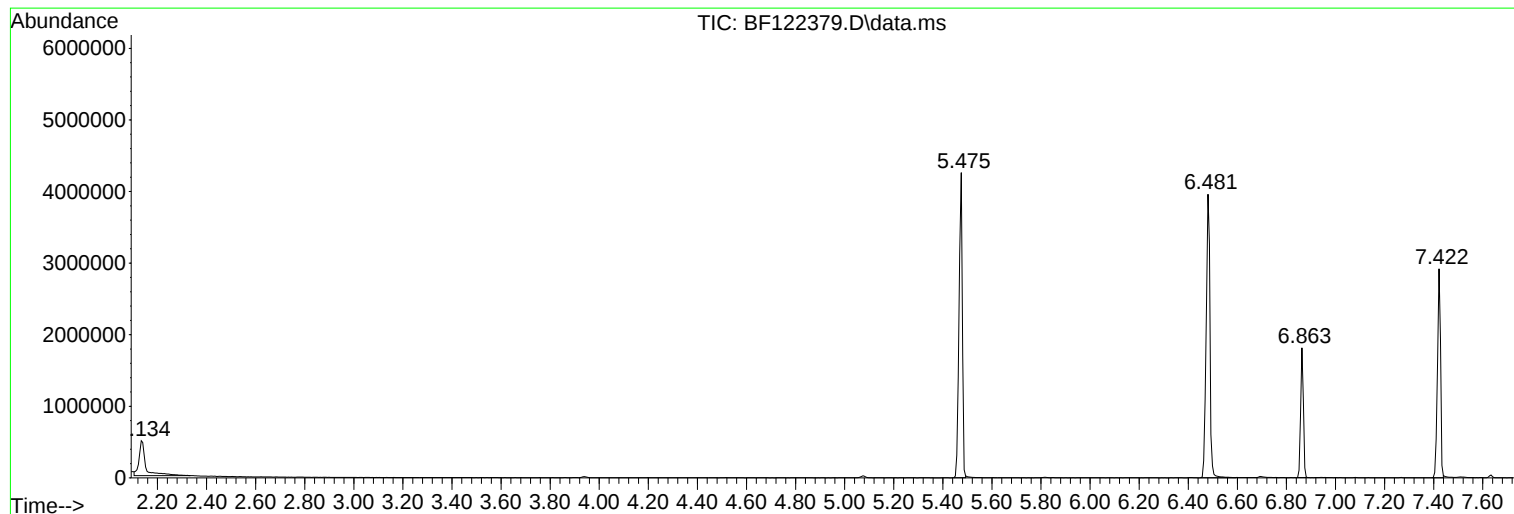
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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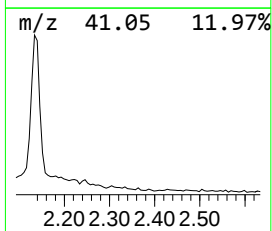
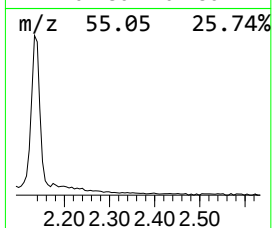
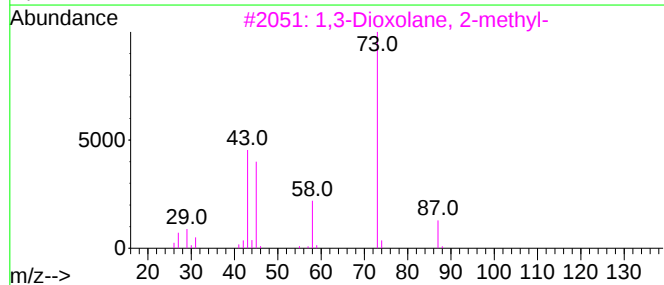
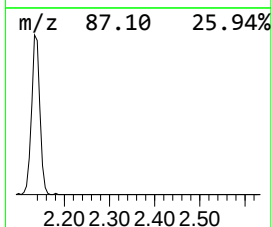
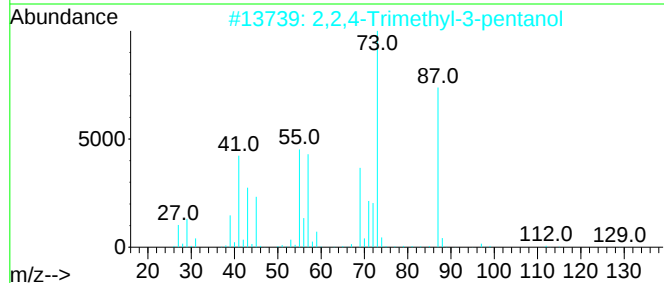
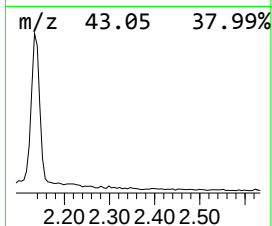
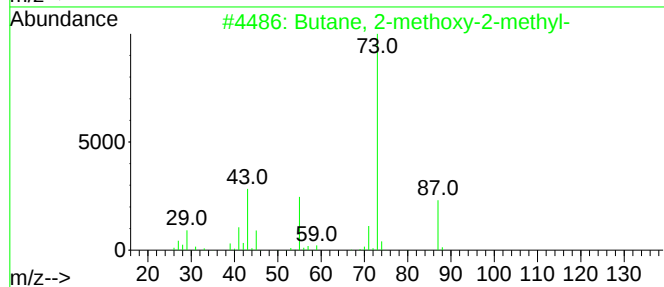
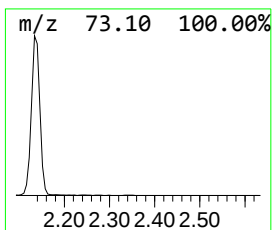
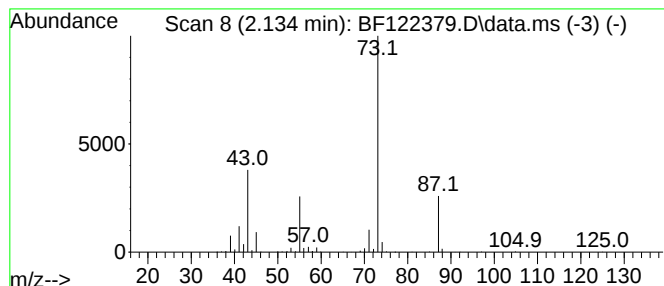
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	13.54 ng	952933	1,4-Dichlorobenzene-d4	6.863

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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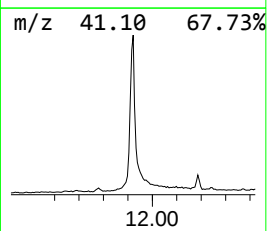
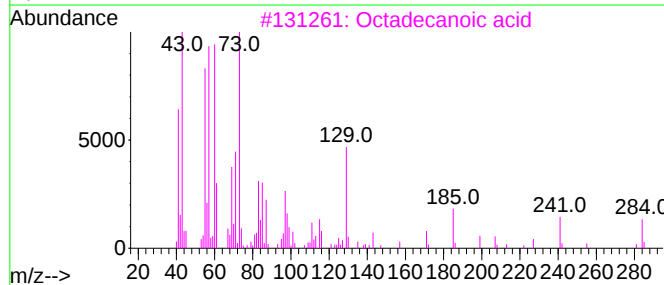
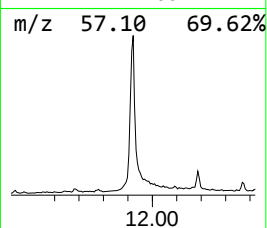
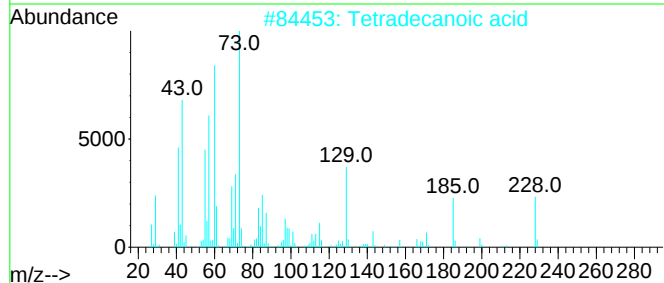
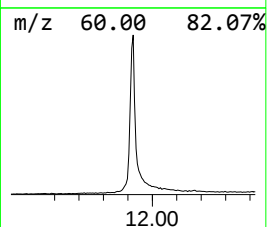
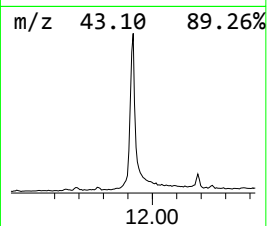
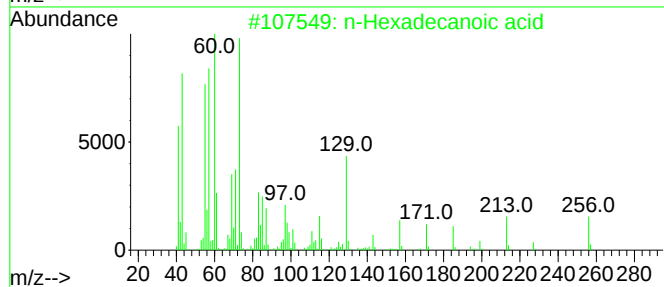
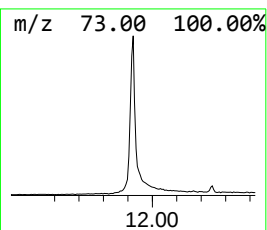
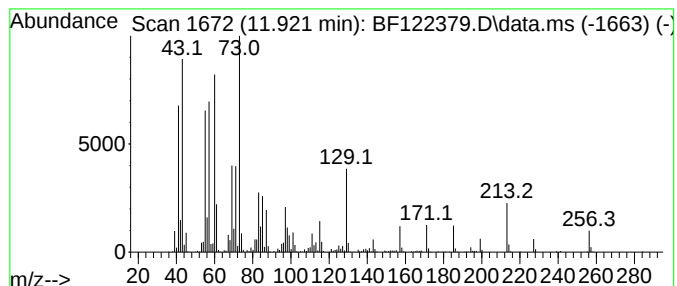
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	25.45 ng	3037460	Phenanthrene-d10	11.386

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			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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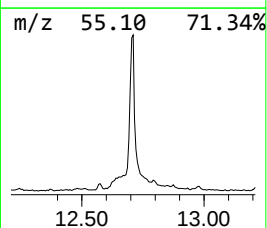
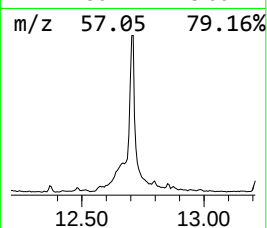
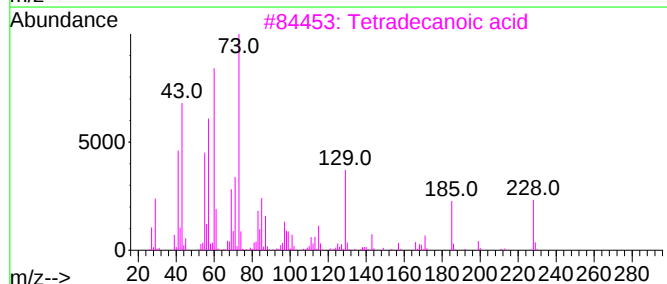
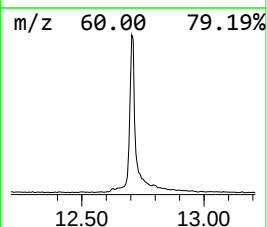
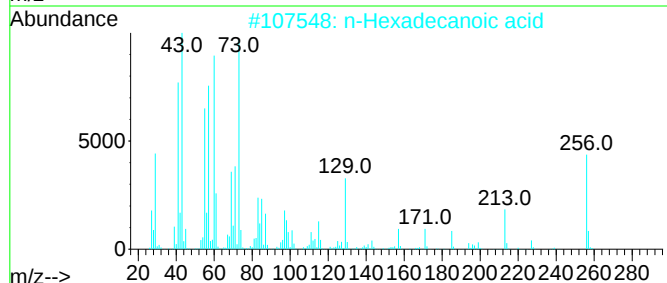
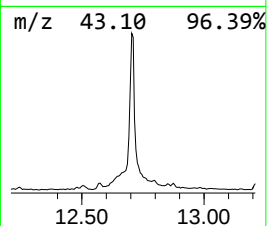
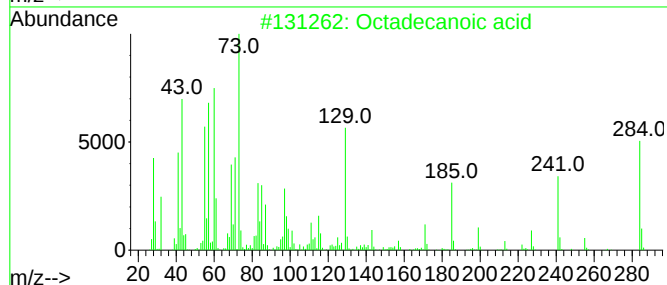
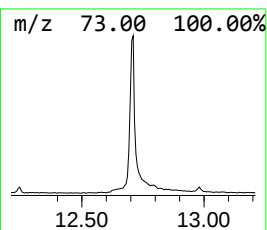
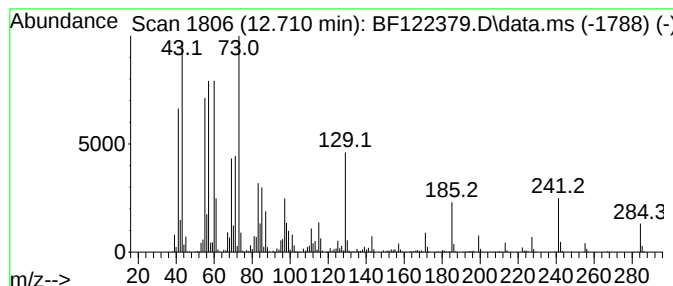
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	36.10 ng	4486080	Chrysene-d12	14.027

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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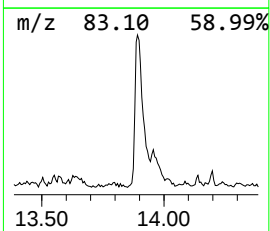
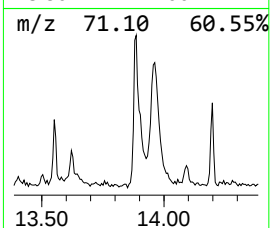
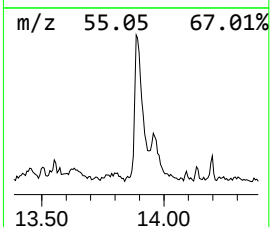
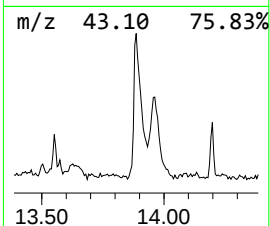
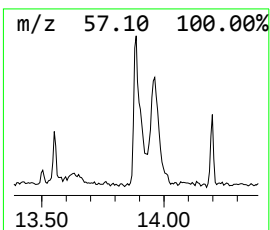
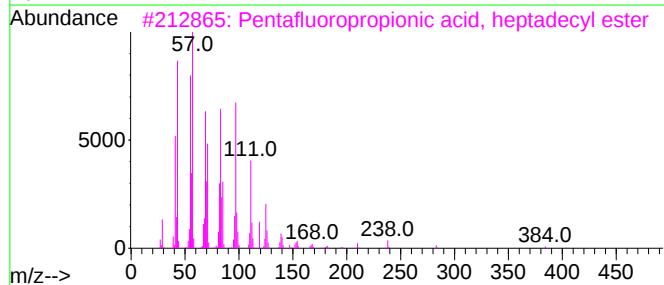
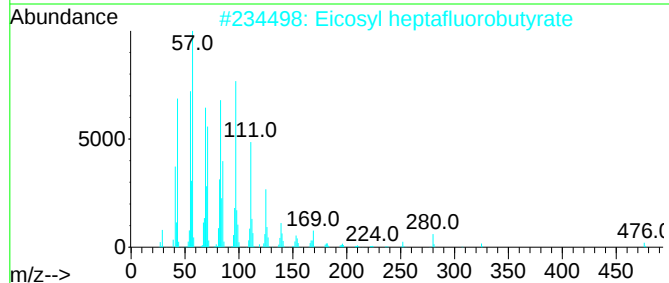
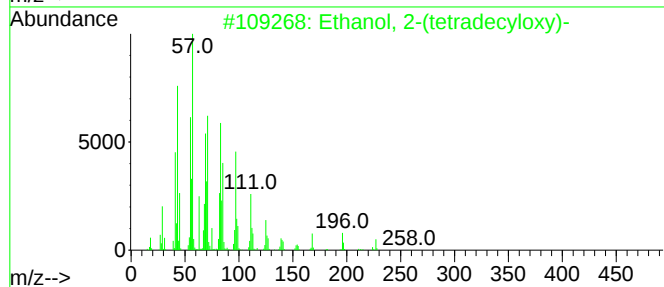
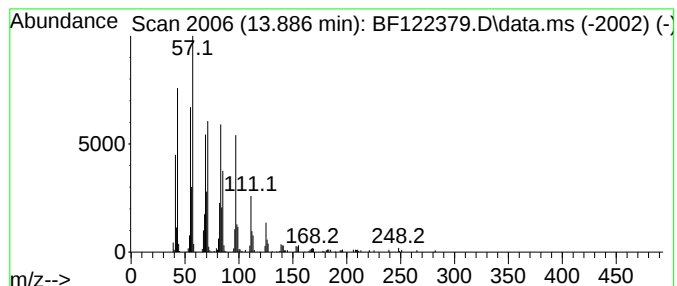
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Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.41 ng	671724	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90



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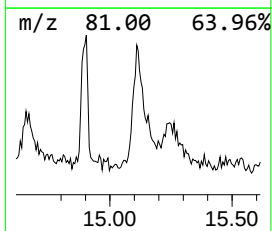
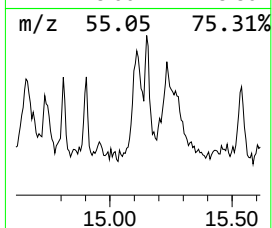
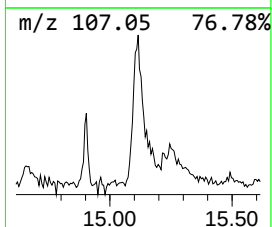
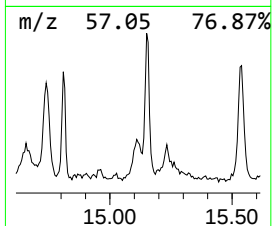
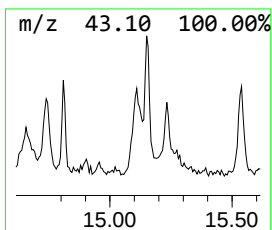
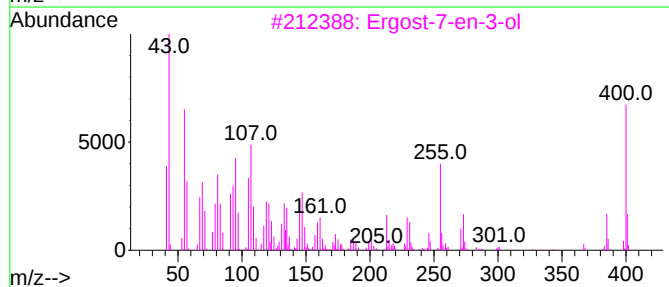
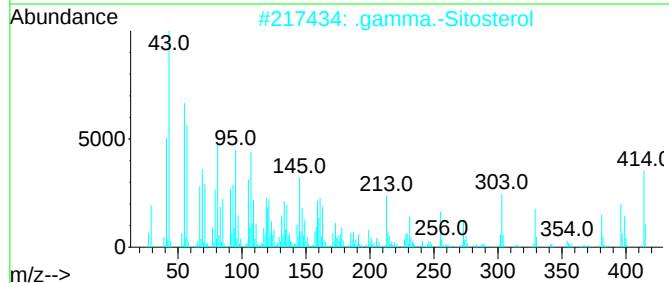
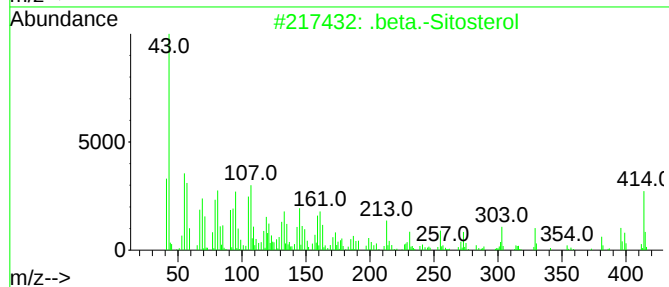
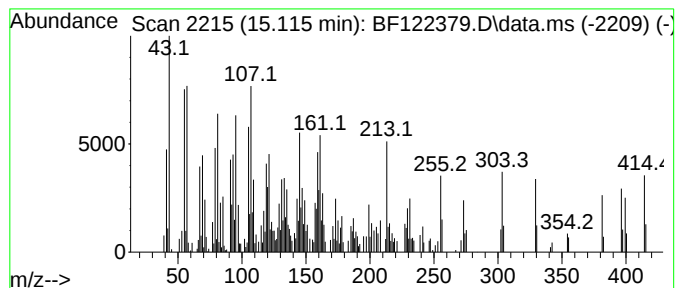
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	4.13 ng	502692	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
3			Ergost-7-en-3-ol	400	C28H48O	116179-22-7	51
4			5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	38
5			Campesterol	400	C28H48O	000474-62-4	35



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ClientSampleId :
R-LA-2-5-WC

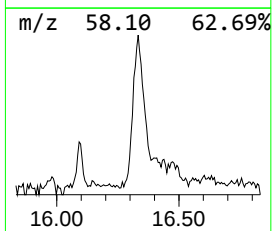
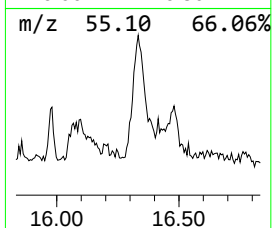
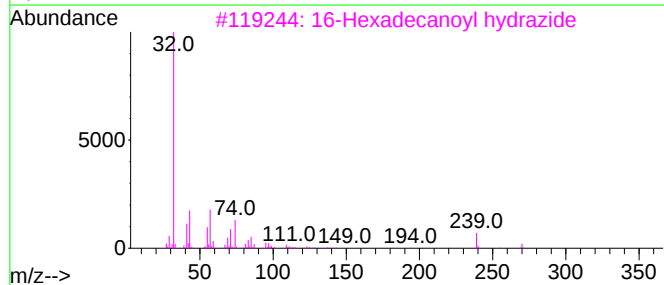
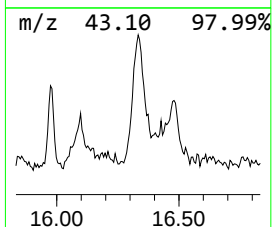
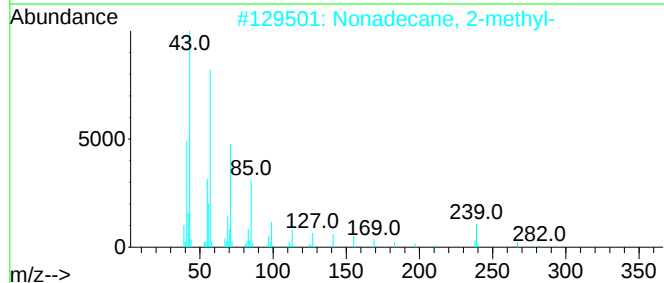
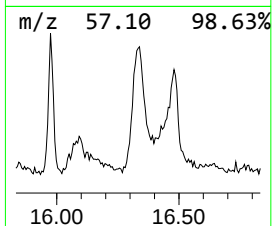
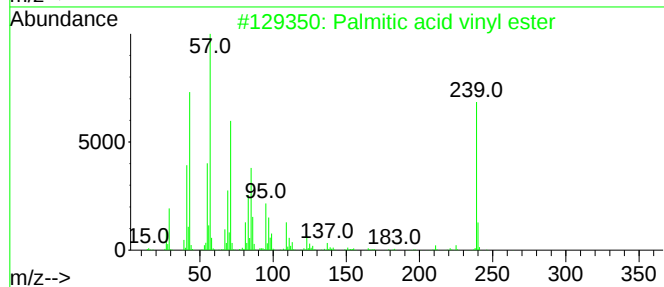
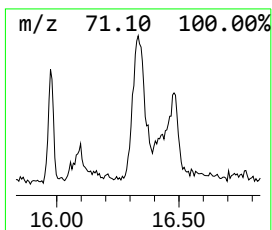
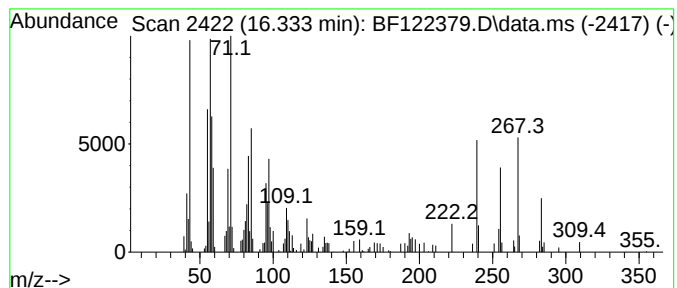
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown16.33 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	3.84 ng	467273	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	43
2			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	43
3			16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	38
4			Nonadecane	268	C19H40	000629-92-5	30
5			Eicosane	282	C20H42	000112-95-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111920\
Data File : BF122379.D
Acq On : 19 Nov 2020 14:29
Operator : JU/CG
Sample : L4797-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-2-5-WC

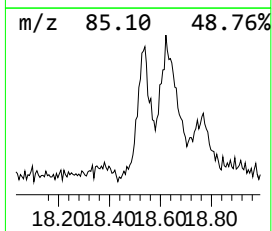
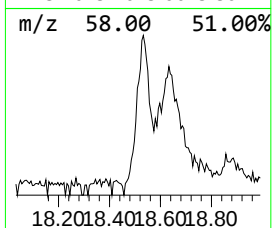
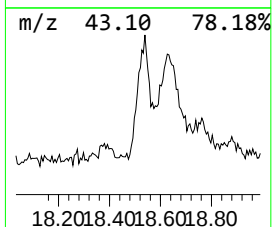
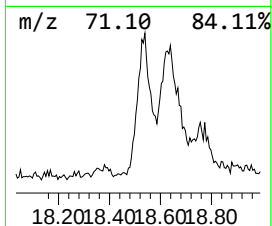
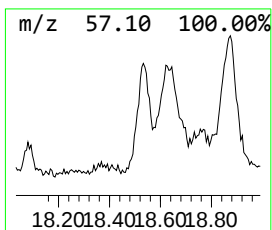
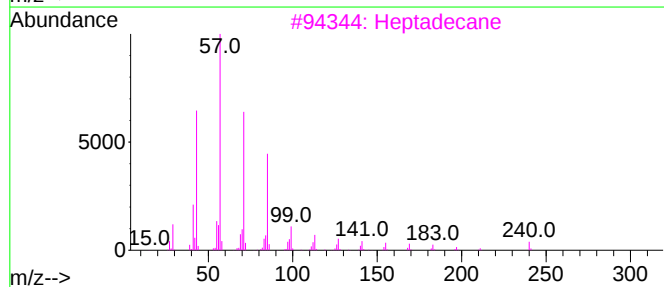
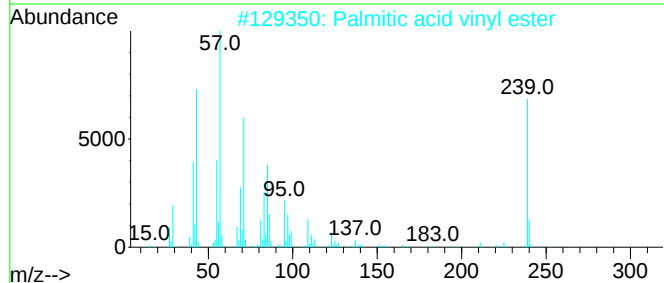
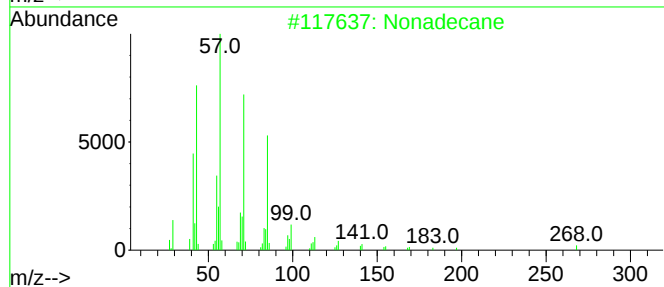
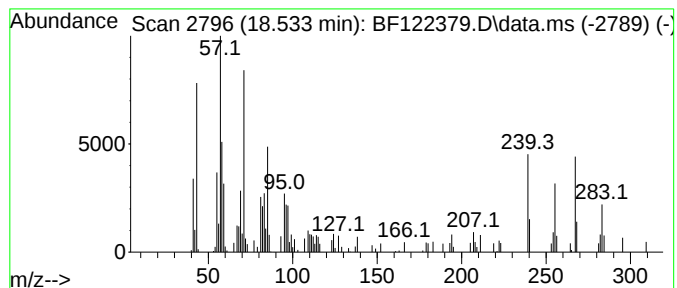
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown18.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.533	2.30 ng	279115	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	38
2			Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	38
3			Heptadecane	240	C17H36	000629-78-7	38
4			Hentriacontane	437	C31H64	000630-04-6	35
5			Eicosane	282	C20H42	000112-95-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111920\
Data File : BF122379.D
Acq On : 19 Nov 2020 14:29
Operator : JU/CG
Sample : L4797-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-2-5-WC

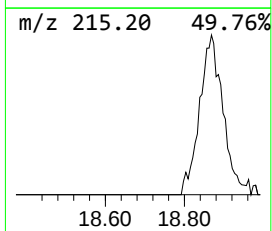
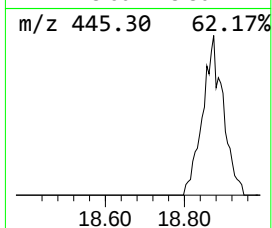
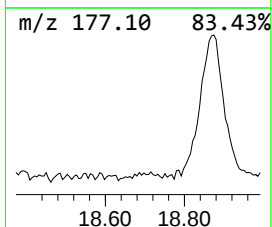
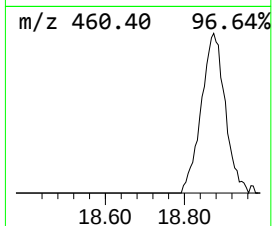
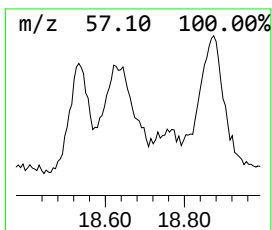
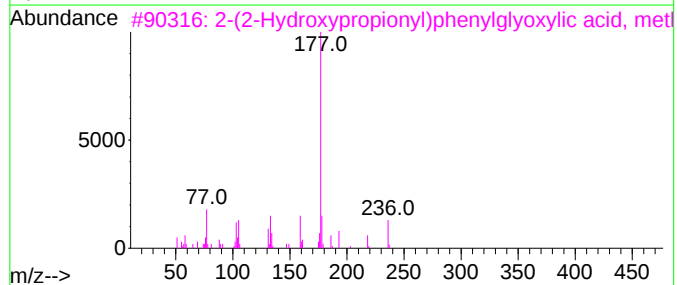
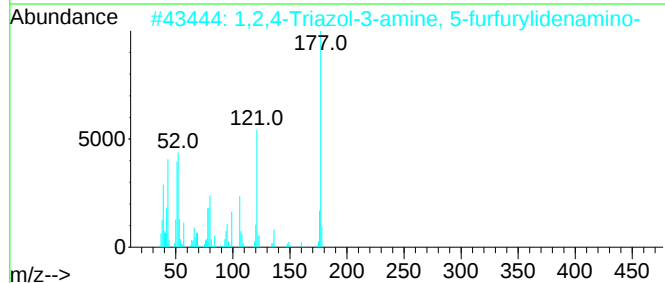
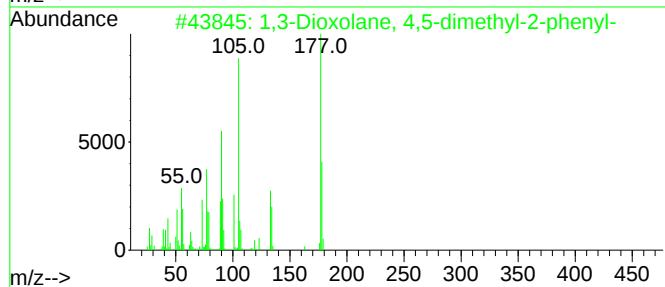
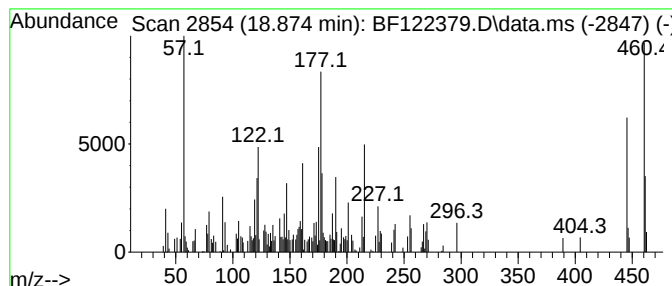
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown18.87 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.874	5.14 ng	625115	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 4,5-dimethyl-2-ph...	178	C11H14O2	004359-31-3	11
2			1,2,4-Triazol-3-amine, 5-furfury...	177	C7H7N5O	1000259-34-3	11
3			2-(2-Hydroxypropionyl)phenylglyo...	236	C12H12O5	100519-35-5	11
4			Benzofuran-2-one, 4-amino-2,3-di...	177	C10H11NO2	1000129-51-7	11
5			Silane, diphenyldecyloxy(3-ethyl...	460	C30H40O2Si	1000367-46-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111920\
Data File : BF122379.D
Acq On : 19 Nov 2020 14:29
Operator : JU/CG
Sample : L4797-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-2-5-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	13.5	ng	952933	1	6.863	1407230	20.0
n-Hexadecanoic ...	11.921	25.4	ng	3037460	4	11.386	2386960	20.0
Octadecanoic acid	12.710	36.1	ng	4486080	5	14.027	2485190	20.0
Ethanol, 2-(tet...	13.886	5.4	ng	671724	5	14.027	2485190	20.0
.beta.-Sitosterol	15.115	4.1	ng	502692	6	15.498	2432150	20.0
unknown16.33	16.333	3.8	ng	467273	6	15.498	2432150	20.0
unknown18.53	18.533	2.3	ng	279115	6	15.498	2432150	20.0
unknown18.87	18.874	5.1	ng	625115	6	15.498	2432150	20.0