

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
 Data File : BF122912.D
 Acq On : 4 Jan 2021 17:01
 Operator : JU/CG
 Sample : L5248-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VR16125

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	495	498	504	rBV	22468	27424	1.93%	0.168%
2	5.434	566	569	590	rBV	807012	925877	65.09%	5.662%
3	6.457	739	743	763	rBV	828953	1003677	70.56%	6.138%
4	6.816	801	804	816	rBV	632397	600697	42.23%	3.674%
5	7.245	874	877	887	rBV	37693	62483	4.39%	0.382%
6	7.381	897	900	912	rBV	617456	584059	41.06%	3.572%
7	8.104	1020	1023	1041	rVB	785098	760471	53.46%	4.651%
8	9.181	1203	1206	1217	rBV	1141125	1015545	71.40%	6.211%
9	9.581	1270	1274	1277	rBV	50498	43688	3.07%	0.267%
10	9.863	1319	1322	1332	rVB	1005740	926389	65.13%	5.666%
11	10.628	1419	1452	1453	rBV2	111613	453807	31.90%	2.775%
12	10.657	1453	1457	1461	rBV	889853	885098	62.23%	5.413%
13	10.728	1466	1469	1470	rBV2	48990	50713	3.57%	0.310%
14	10.804	1476	1482	1484	rBV	278906	450039	31.64%	2.752%
15	11.022	1517	1519	1525	rVB2	24573	26228	1.84%	0.160%
16	11.357	1572	1576	1584	rBV	1136404	973833	68.46%	5.956%
17	11.880	1644	1665	1677	rBV3	397982	1422404	100.00%	8.699%
18	12.033	1679	1691	1706	rVB4	86198	391317	27.51%	2.393%
19	12.333	1736	1742	1748	rBV8	9835	25489	1.79%	0.156%
20	12.669	1796	1799	1806	rVB	56702	64213	4.51%	0.393%
21	12.945	1841	1846	1850	rBV	1613441	1394638	98.05%	8.529%
22	13.221	1886	1893	1901	rVB	203346	414469	29.14%	2.535%
23	13.427	1923	1928	1932	rVB4	17229	23036	1.62%	0.141%
24	13.498	1938	1940	1946	rVB5	12444	18253	1.28%	0.112%
25	13.798	1986	1991	1994	rBV	45735	59250	4.17%	0.362%
26	13.833	1994	1997	2000	rVV	60945	67801	4.77%	0.415%
27	13.869	2000	2003	2010	rVB	228151	244789	17.21%	1.497%
28	13.986	2016	2023	2024	rBV	231988	314209	22.09%	1.922%
29	14.010	2024	2027	2036	rVB	1171455	1134037	79.73%	6.935%
30	14.468	2102	2105	2110	rVB2	25481	23009	1.62%	0.141%
31	14.563	2116	2121	2127	rBV	199332	323047	22.71%	1.976%
32	14.721	2145	2148	2154	rVB7	26298	40169	2.82%	0.246%
33	14.774	2154	2157	2162	rVB	30400	33890	2.38%	0.207%
34	14.851	2167	2170	2175	rVB3	22627	26433	1.86%	0.162%
35	15.115	2211	2215	2216	rBV	61423	67961	4.78%	0.416%
36	15.139	2216	2219	2228	rVB	96212	167272	11.76%	1.023%

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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-BF120520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.486	2273	2278	2289	rVB	789277	1033146	72.63%	6.318%
38	15.786	2324	2329	2342	rVB4	29284	93690	6.59%	0.573%
39	15.921	2348	2352	2357	rBV2	40353	57259	4.03%	0.350%
40	16.421	2434	2437	2444	rVB2	29309	49673	3.49%	0.304%
41	16.527	2450	2455	2462	rVB6	20509	49593	3.49%	0.303%
42	16.933	2520	2524	2529	rBV8	9712	22258	1.56%	0.136%

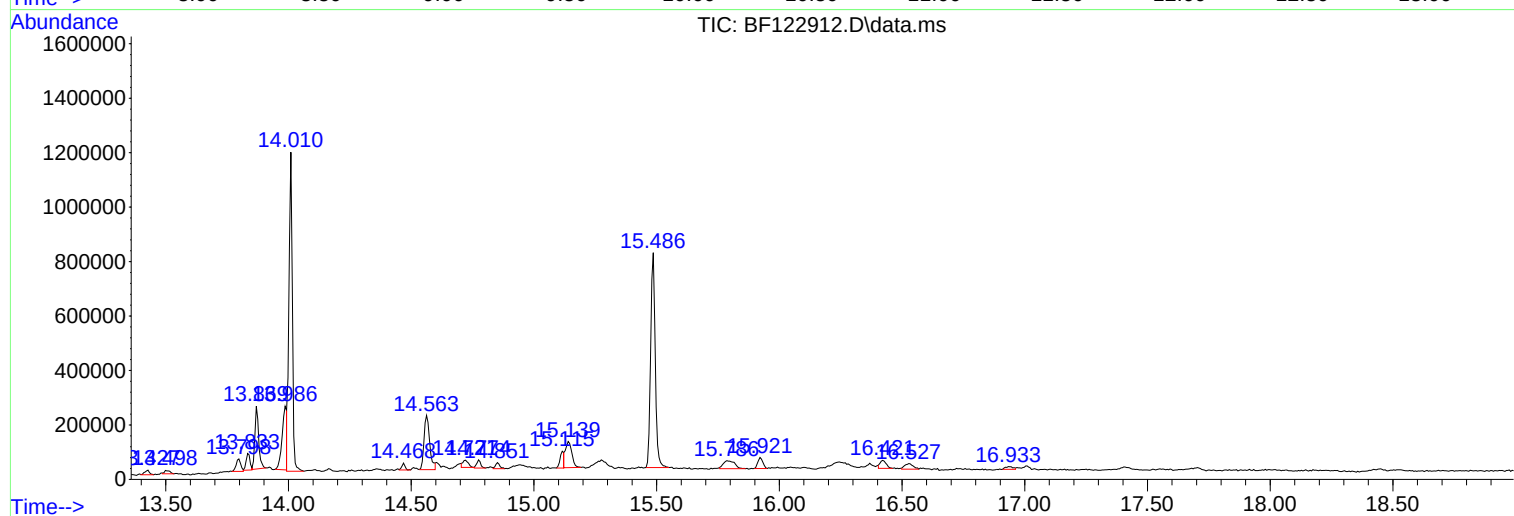
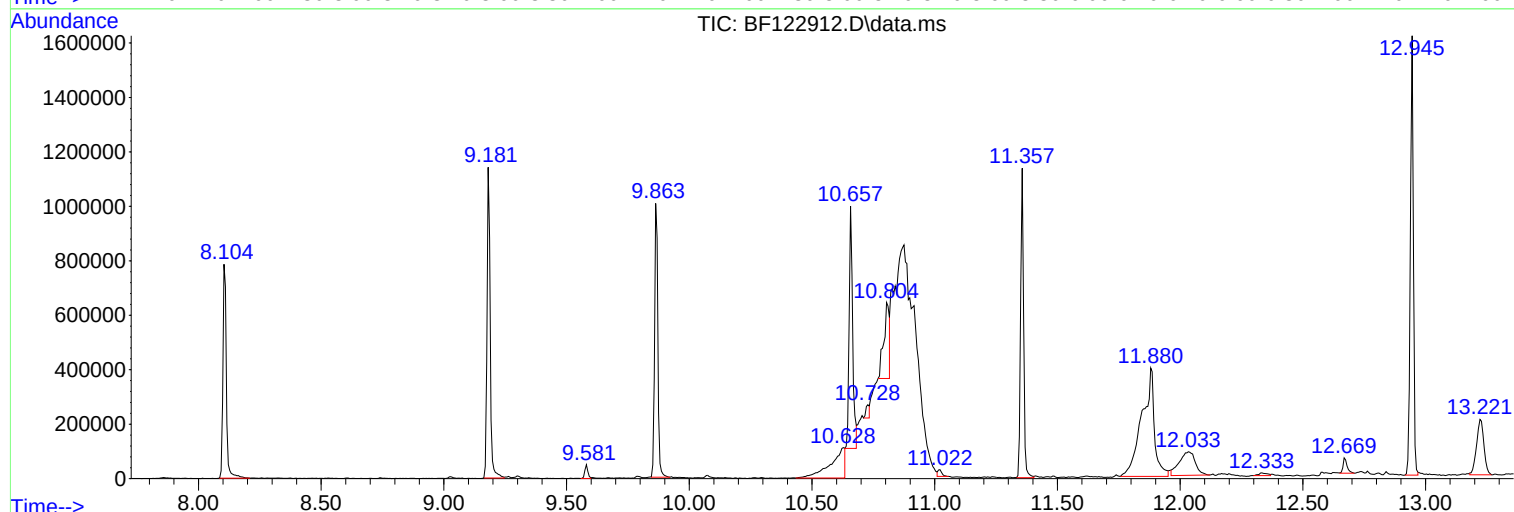
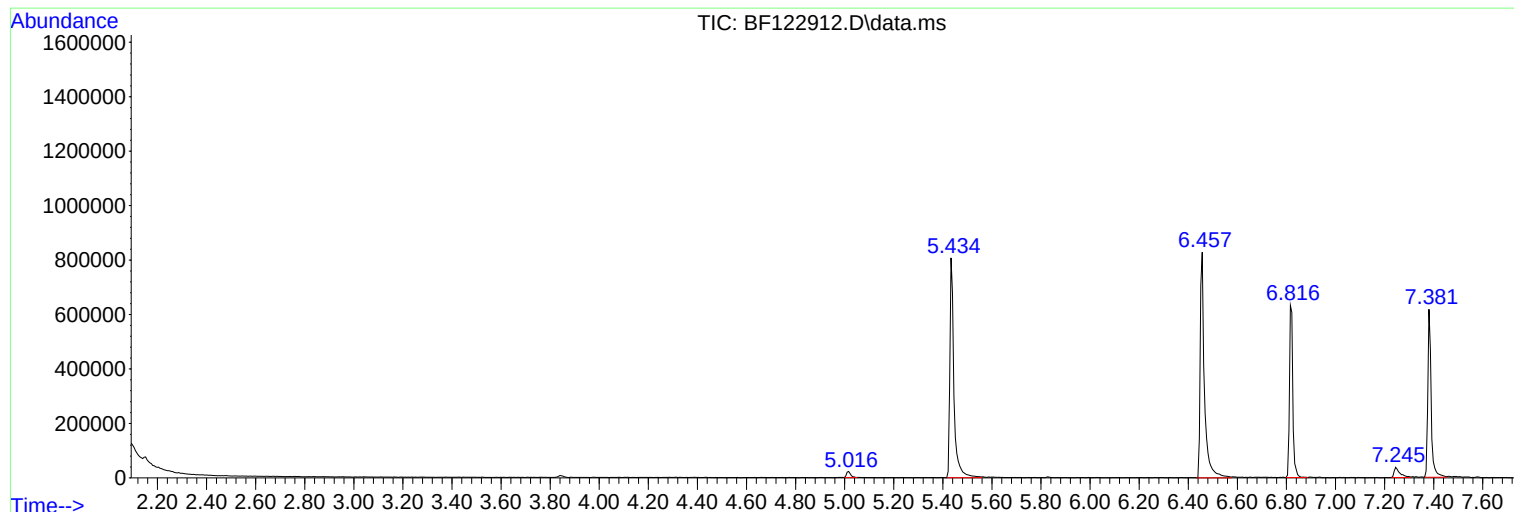
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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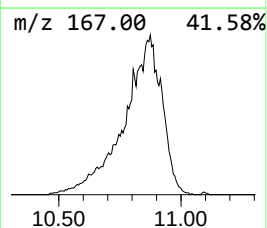
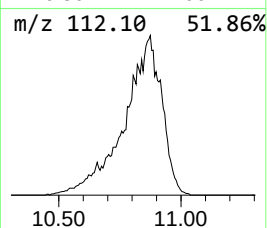
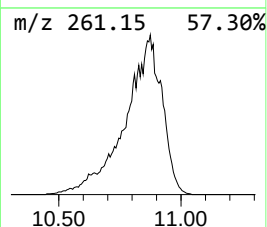
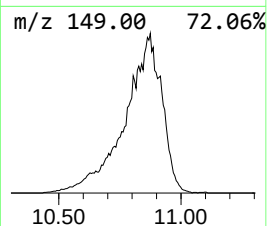
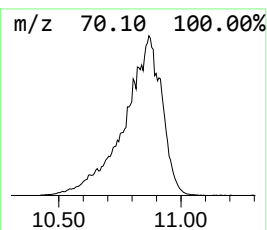
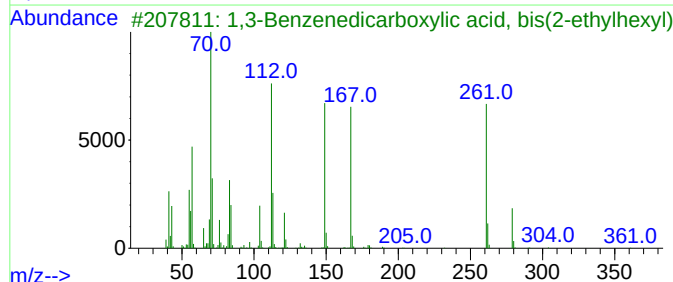
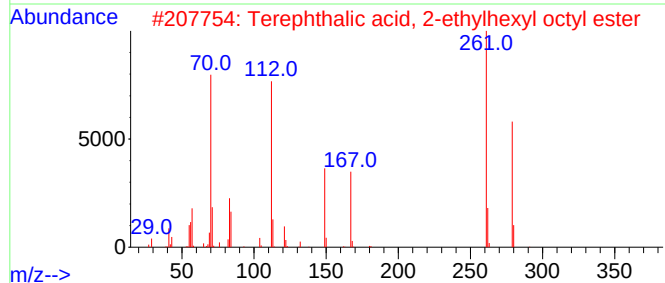
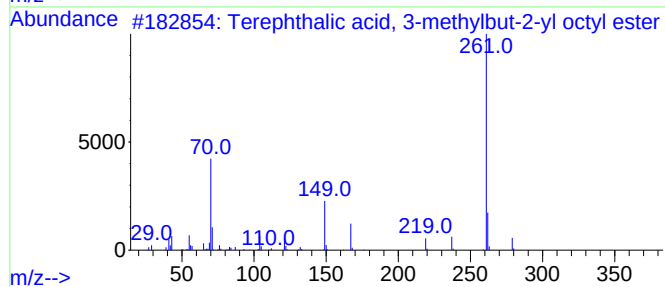
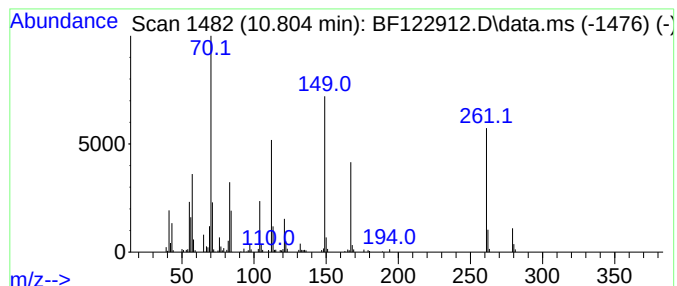
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Terephthalic acid, 3-methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	9.24 ng	450039	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	47
5			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	43



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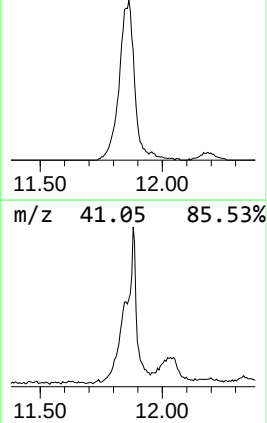
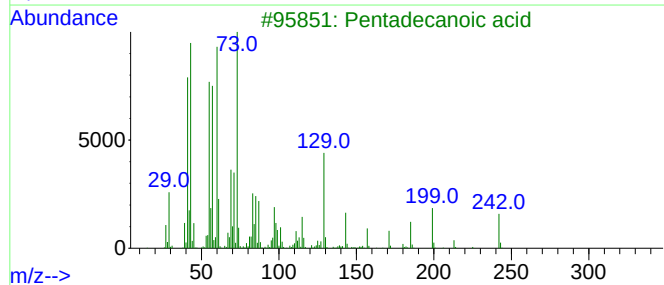
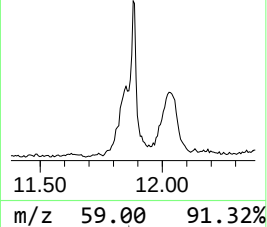
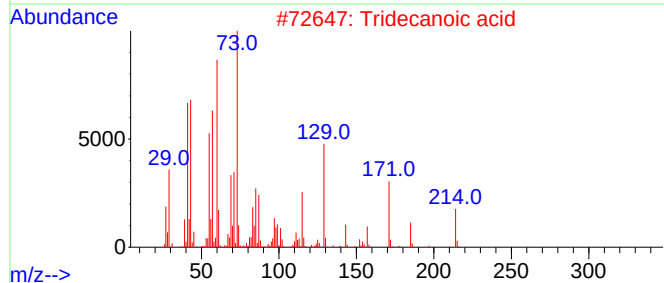
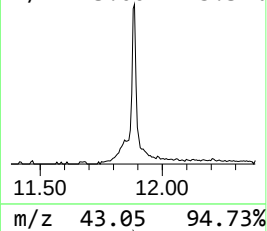
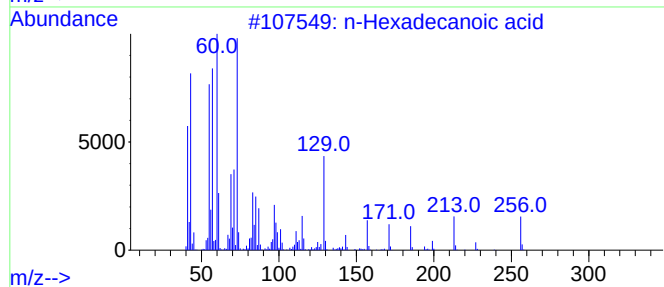
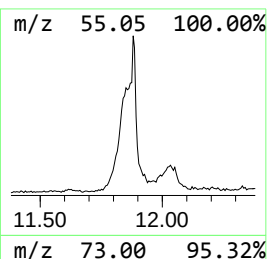
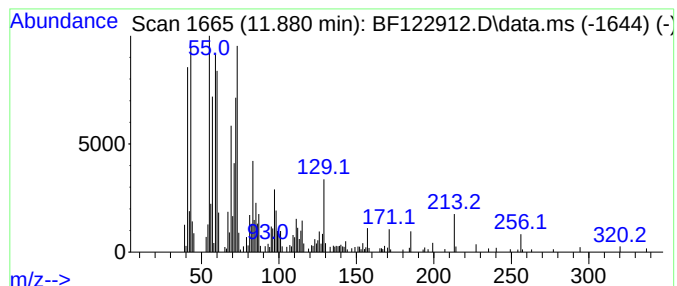
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	29.21 ng	1422400	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	84
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38
5			N-(5-Oxo-tetrahydro-furan-2-ylme...	157	C7H11NO3	1000188-71-2	38



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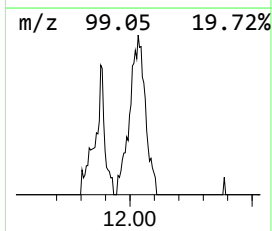
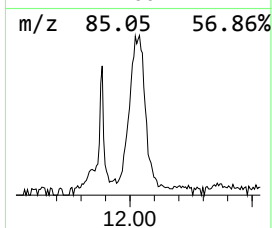
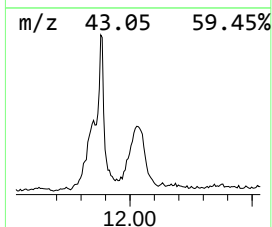
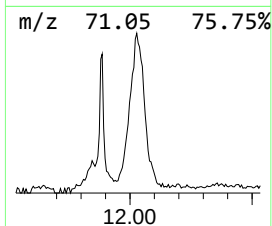
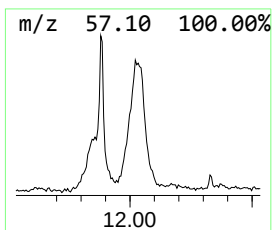
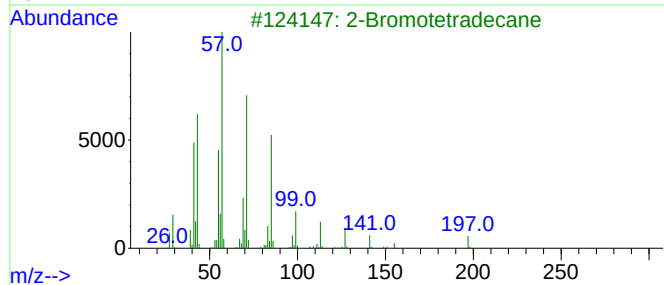
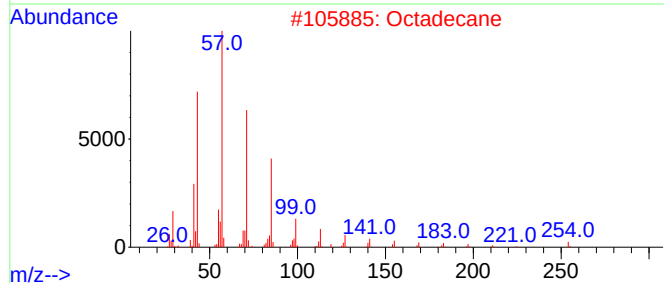
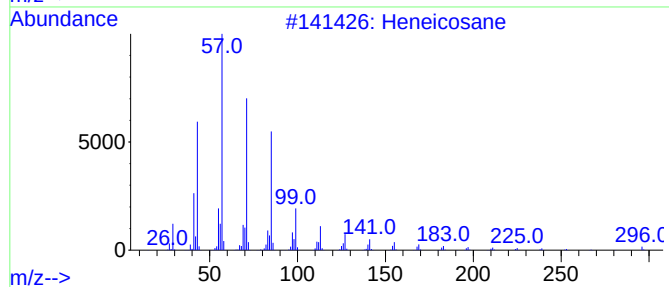
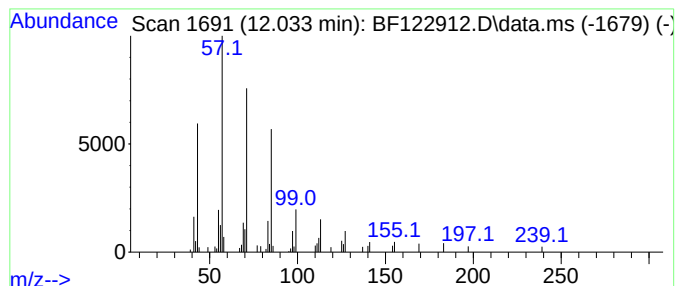
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	8.04 ng	391317	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octadecane	254	C18H38	000593-45-3	90
3			2-Bromotetradecane	276	C14H29Br	074036-95-6	90
4			Heptadecane	240	C17H36	000629-78-7	86
5			Hexadecane	226	C16H34	000544-76-3	78



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ALS Vial : 5 Sample Multiplier: 1

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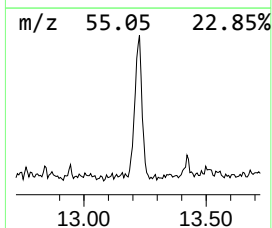
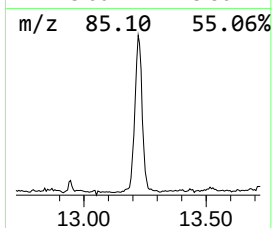
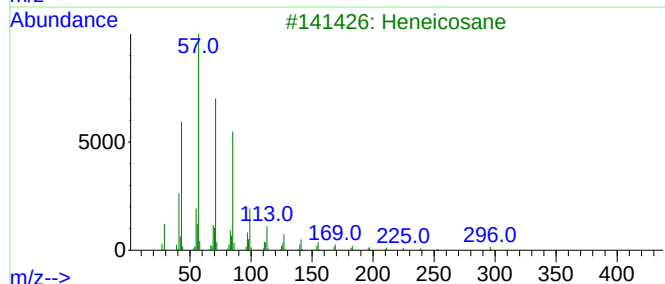
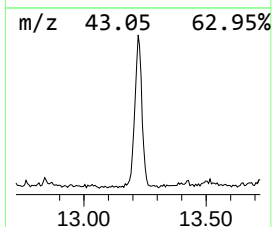
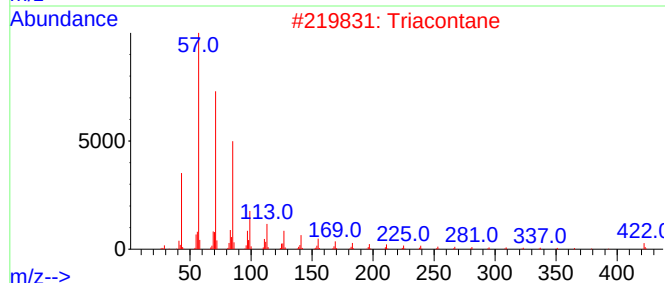
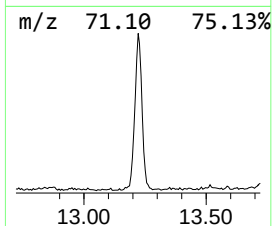
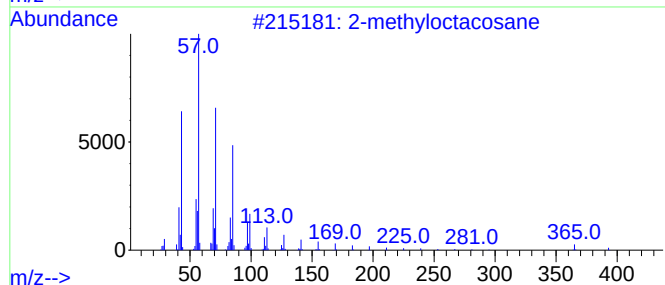
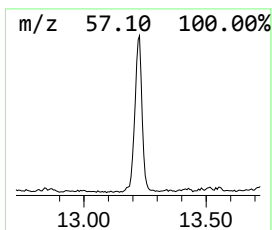
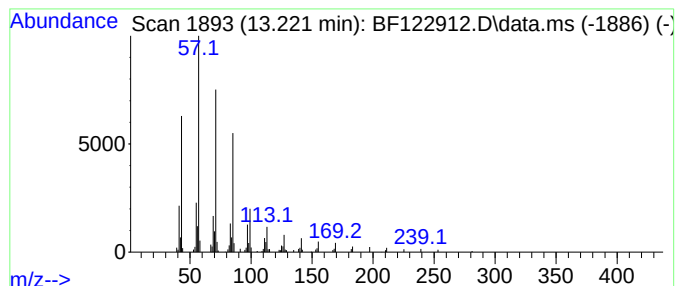
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	7.31 ng	414469	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Triacotane	422	C30H62	000638-68-6	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91



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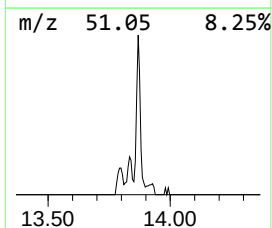
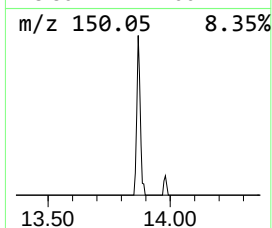
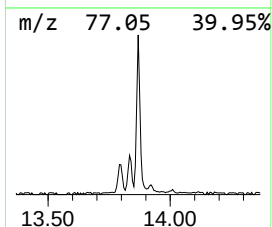
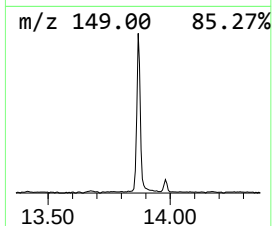
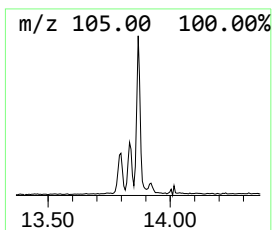
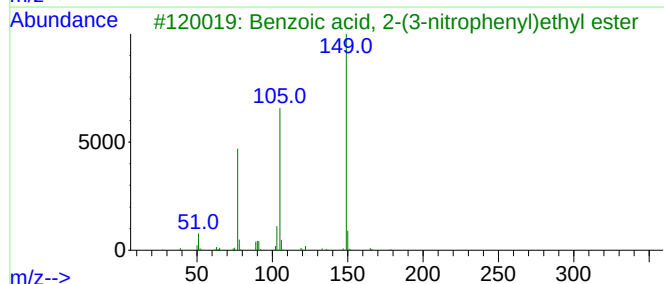
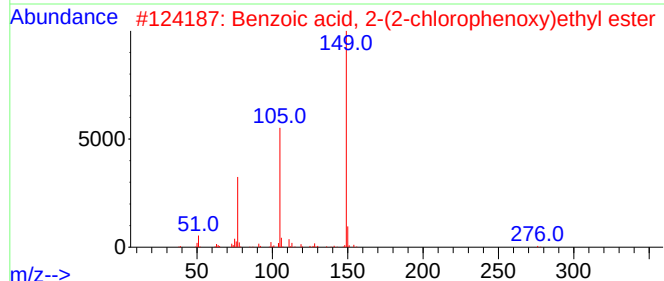
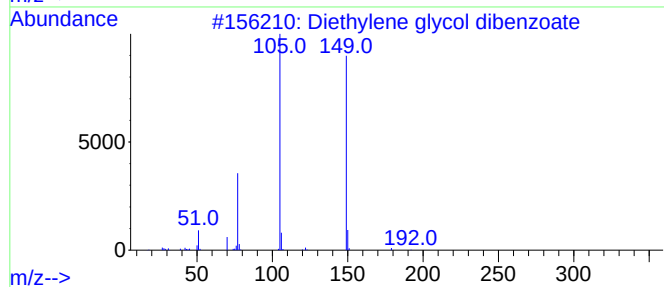
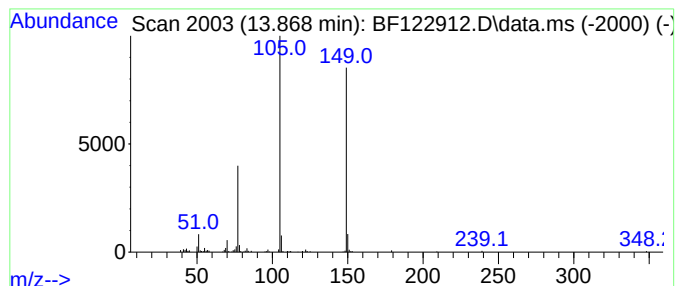
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	4.32 ng	244789	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2			Benzoic acid, 2-(2-chlorophenoxy)...	276	C15H13ClO3	1000368-25-9	72
3			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
4			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
5			Phthalic acid, 2-chloropropyl he...	466	C27H43ClO4	1000356-83-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
Data File : BF122912.D
Acq On : 4 Jan 2021 17:01
Operator : JU/CG
Sample : L5248-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VR16125

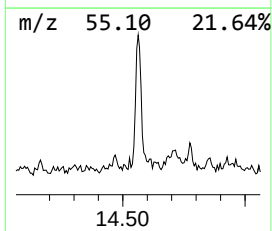
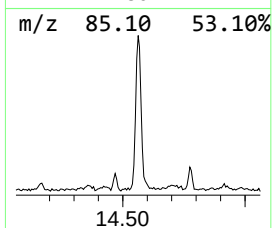
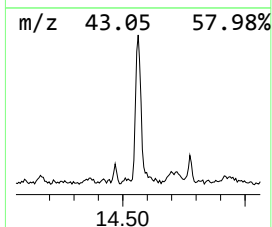
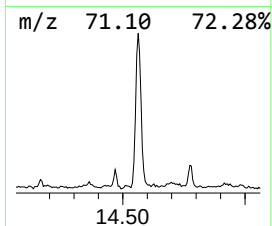
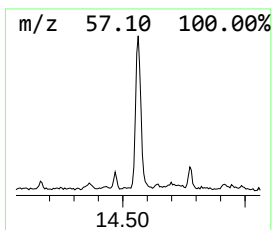
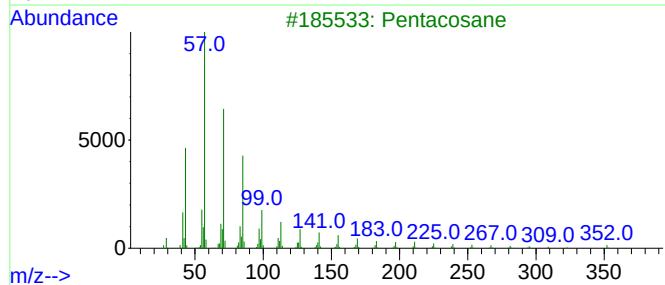
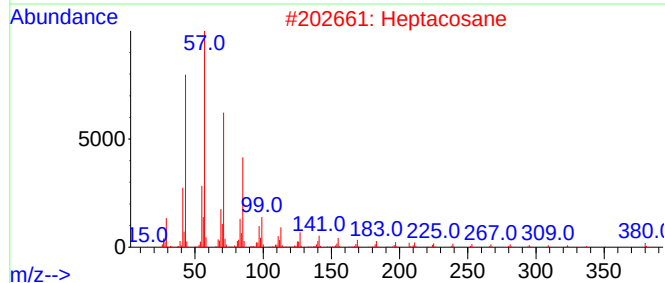
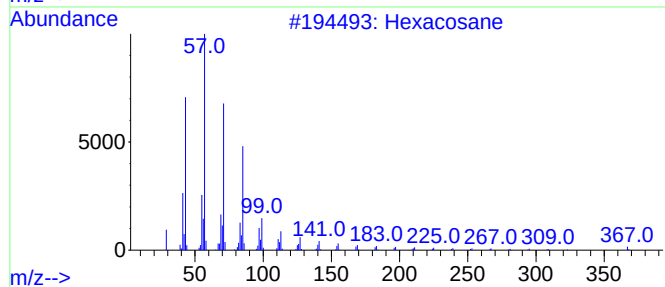
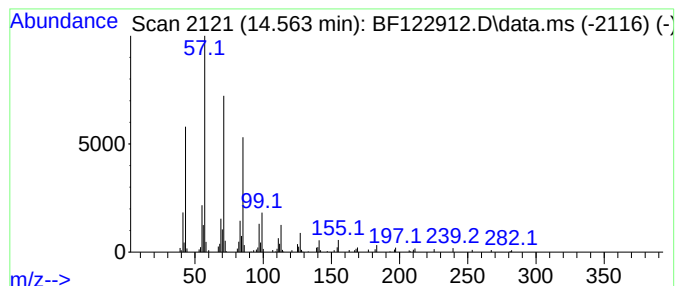
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	5.70 ng	323047	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Heptacosane	380	C27H56	000593-49-7	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
Data File : BF122912.D
Acq On : 4 Jan 2021 17:01
Operator : JU/CG
Sample : L5248-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VR16125

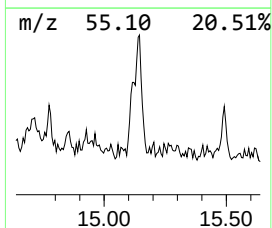
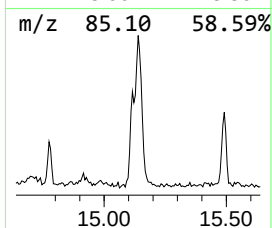
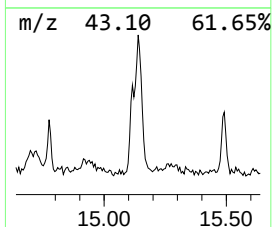
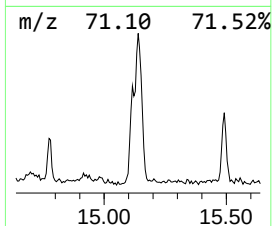
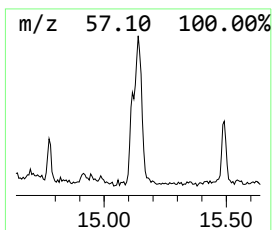
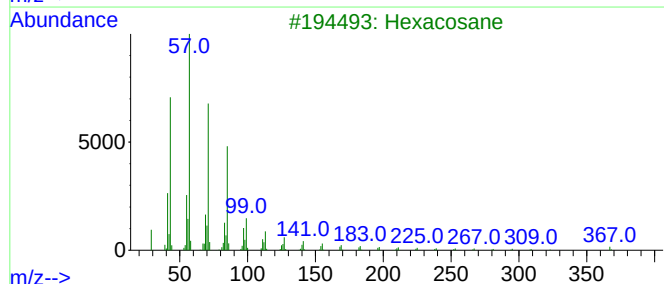
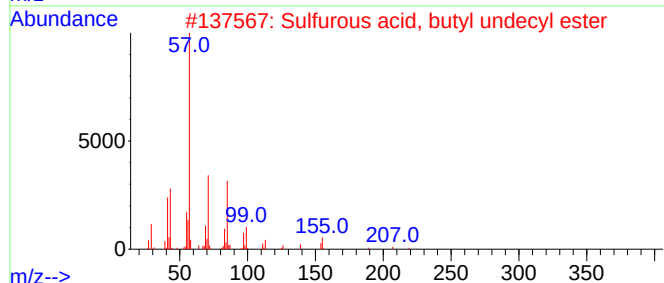
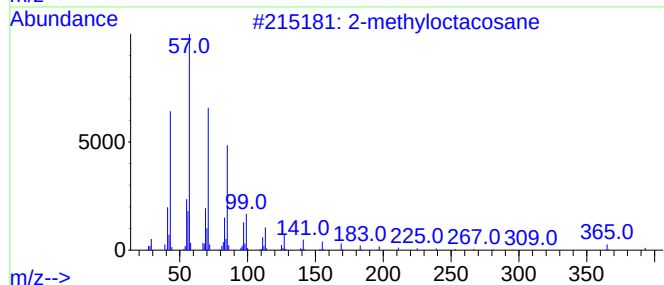
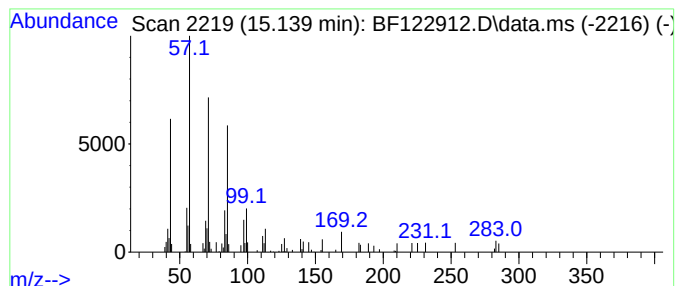
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl undec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	3.24 ng	167272	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane			408	C29H60	1000376-72-8	87
2	Sulfurous acid, butyl undecyl ester			292	C15H32O3S	1000309-17-8	80
3	Hexacosane			366	C26H54	000630-01-3	76
4	Sulfurous acid, butyl dodecyl ester			306	C16H34O3S	1000309-17-9	72
5	Heneicosane			296	C21H44	000629-94-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010421\
Data File : BF122912.D
Acq On : 4 Jan 2021 17:01
Operator : JU/CG
Sample : L5248-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VR16125

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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
Terephthalic ac...	10.804	9.2	ng	450039	4	11.357	973833	20.0
n-Hexadecanoic ...	11.880	29.2	ng	1422400	4	11.357	973833	20.0
Heneicosane	12.033	8.0	ng	391317	4	11.357	973833	20.0
2-methyloctacosane	13.222	7.3	ng	414469	5	14.010	1134040	20.0
Diethylene glyc...	13.868	4.3	ng	244789	5	14.010	1134040	20.0
Hexacosane	14.563	5.7	ng	323047	5	14.010	1134040	20.0
Sulfurous acid,...	15.139	3.2	ng	167272	6	15.486	1033150	20.0