

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
 Data File : BF135759.D
 Acq On : 13 Oct 2023 18:39
 Operator : CG\JU
 Sample : 04844-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-603-COMP-07

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	487	490	500	rBV	82715	126015	5.99%	0.741%
2	5.375	555	559	581	rBV	1712177	2103454	100.00%	12.374%
3	6.387	728	731	750	rBV	2011097	2003049	95.23%	11.783%
4	6.734	787	790	801	rBV	822173	734683	34.93%	4.322%
5	7.304	884	887	901	rBV	1456801	1302000	61.90%	7.659%
6	7.992	1001	1004	1005	rBV	55519	42323	2.01%	0.249%
7	8.016	1005	1008	1015	rVB	1084535	902819	42.92%	5.311%
8	8.433	1076	1079	1081	rBV	36219	28246	1.34%	0.166%
9	8.604	1105	1108	1112	rBV	117213	90629	4.31%	0.533%
10	9.092	1187	1191	1201	rBV	2397486	2002583	95.20%	11.780%
11	9.169	1201	1204	1208	rBV	80302	69251	3.29%	0.407%
12	9.210	1208	1211	1214	rBV2	29456	30808	1.46%	0.181%
13	9.704	1292	1295	1299	rBV	43906	34482	1.64%	0.203%
14	9.775	1303	1307	1311	rBV	1055559	899757	42.78%	5.293%
15	10.204	1373	1380	1383	rBV3	36043	36549	1.74%	0.215%
16	10.569	1439	1442	1458	rBV	1327737	1211809	57.61%	7.129%
17	10.680	1458	1461	1466	rVB3	19993	24378	1.16%	0.143%
18	11.269	1558	1561	1564	rBV	1111737	935664	44.48%	5.504%
19	11.292	1564	1565	1570	rVB	90623	77188	3.67%	0.454%
20	11.804	1649	1652	1660	rBV2	213122	224273	10.66%	1.319%
21	11.892	1664	1667	1670	rBV	22989	25002	1.19%	0.147%
22	12.498	1766	1770	1774	rBV	102900	106637	5.07%	0.627%
23	12.598	1783	1787	1792	rBV2	37776	55582	2.64%	0.327%
24	12.727	1804	1809	1816	rVB	101702	115913	5.51%	0.682%
25	12.863	1828	1832	1836	rBV	1866861	1700114	80.82%	10.001%
26	13.351	1910	1915	1921	rBV	220321	208487	9.91%	1.226%
27	13.857	1993	2001	2007	rBV8	25724	78459	3.73%	0.462%
28	13.933	2010	2014	2018	rBV	594827	594026	28.24%	3.494%
29	14.092	2037	2041	2043	rBV	26119	27903	1.33%	0.164%
30	14.398	2090	2093	2097	rBV	38492	38905	1.85%	0.229%
31	14.698	2141	2144	2150	rBV	42037	47169	2.24%	0.277%
32	14.774	2154	2157	2161	rVB	25422	27162	1.29%	0.160%
33	14.992	2190	2194	2197	rBV	29689	47117	2.24%	0.277%
34	15.033	2198	2201	2207	rVB	62349	79900	3.80%	0.470%
35	15.292	2242	2245	2249	rVB	21353	22918	1.09%	0.135%
36	15.357	2253	2256	2260	rVV	27820	30793	1.46%	0.181%

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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-BF101323.M
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37	15.409	2260	2265	2275	rVB	549791	725606	34.50%	4.268%
38	15.845	2335	2339	2346	rBV	40396	67523	3.21%	0.397%
39	16.356	2419	2426	2430	rBV2	31629	59510	2.83%	0.350%
40	16.939	2522	2525	2534	rVB3	29712	60645	2.88%	0.357%

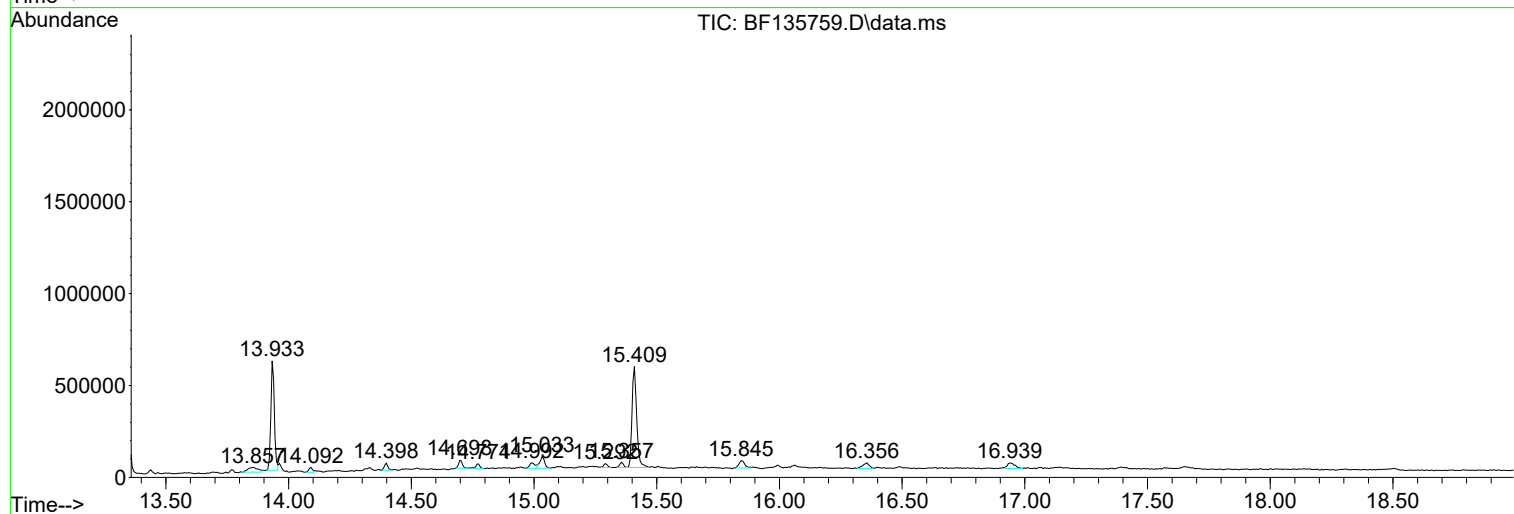
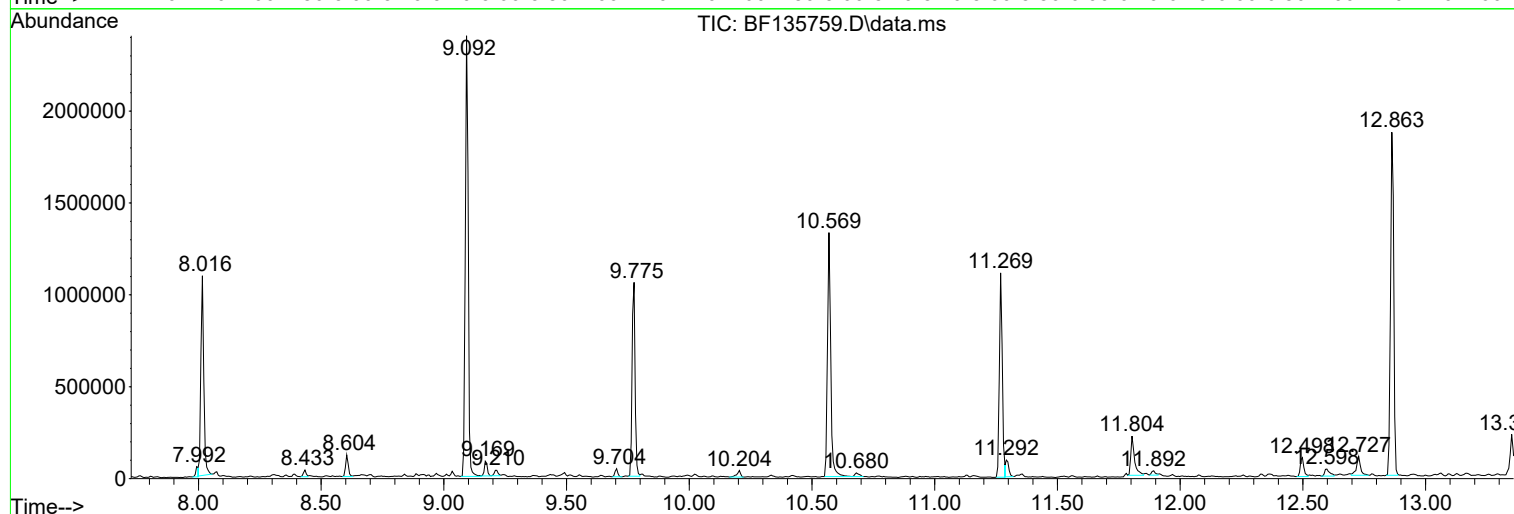
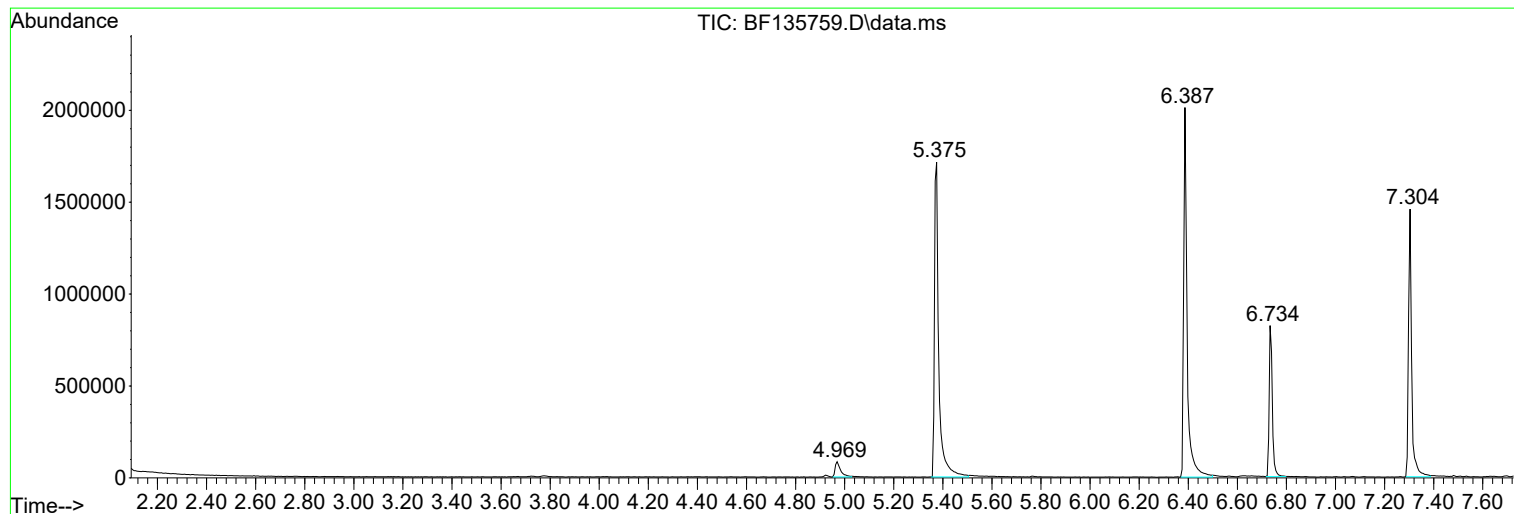
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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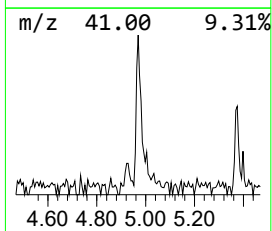
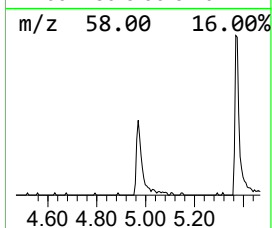
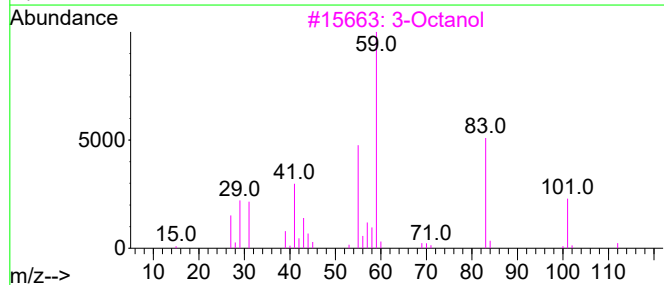
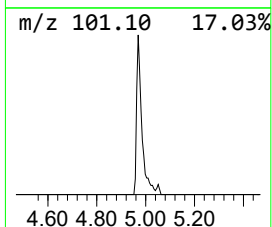
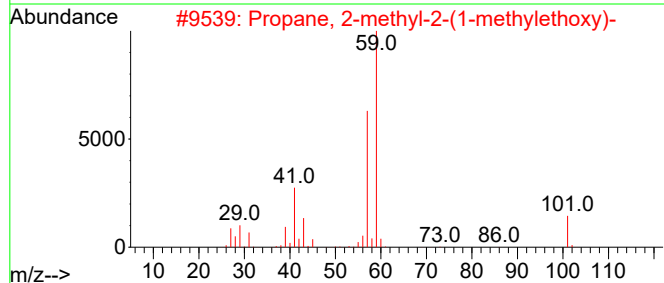
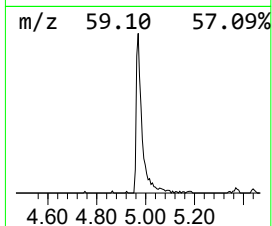
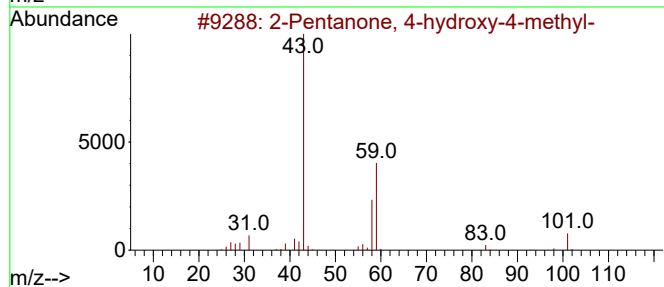
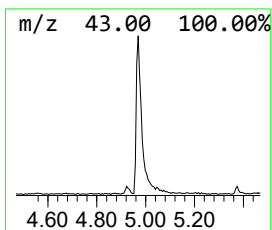
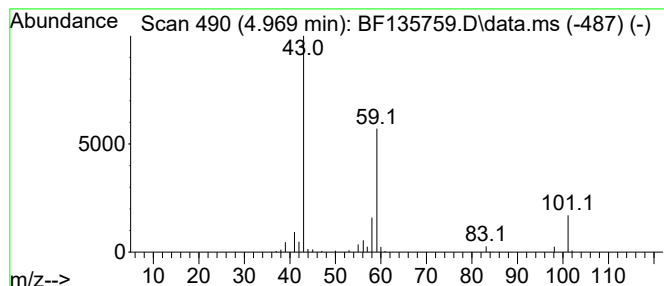
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	3.43 ng	126015	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		



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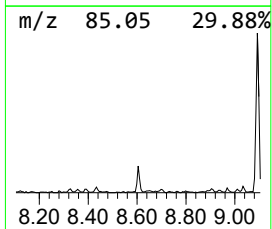
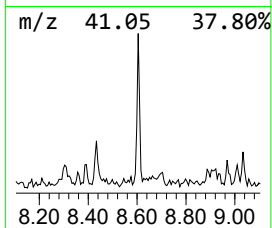
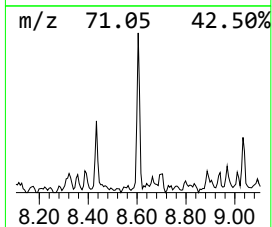
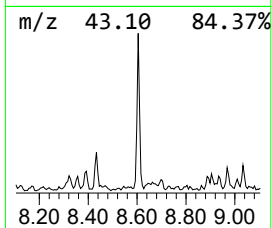
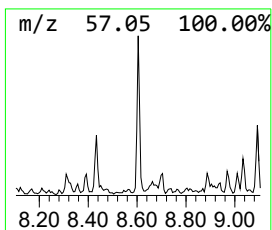
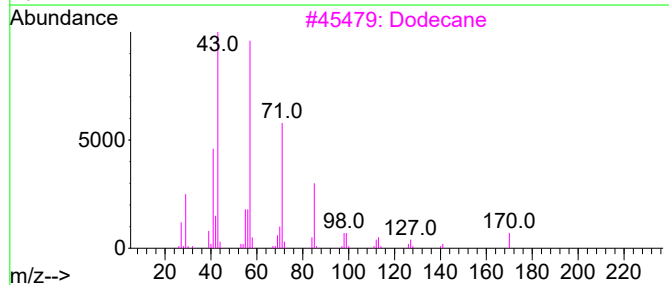
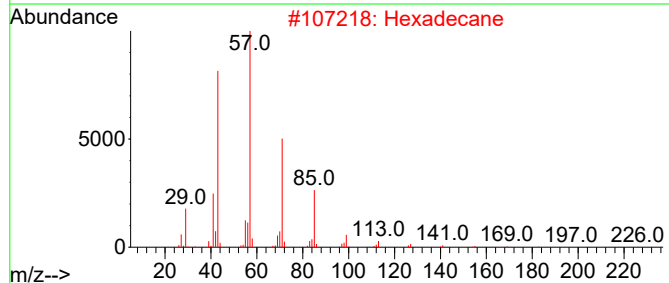
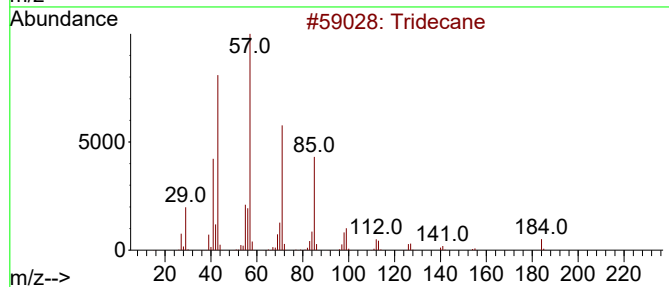
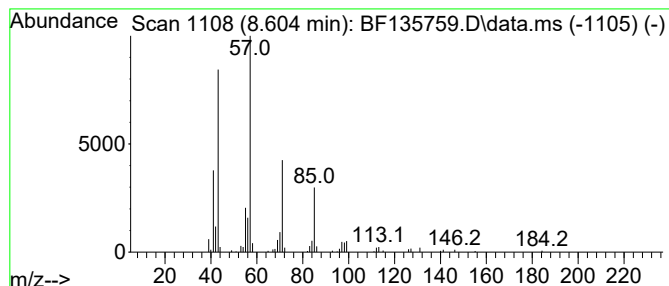
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	2.01 ng	90629	Naphthalene-d8	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Hexadecane	226	C16H34	000544-76-3	90
3			Dodecane	170	C12H26	000112-40-3	78
4			Undecane	156	C11H24	001120-21-4	78
5			Heptadecane	240	C17H36	000629-78-7	72



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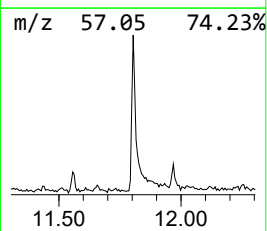
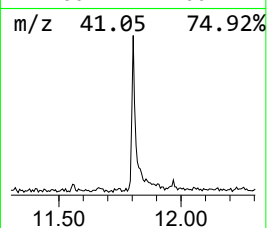
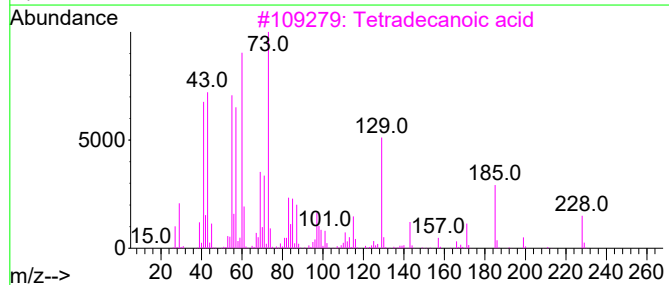
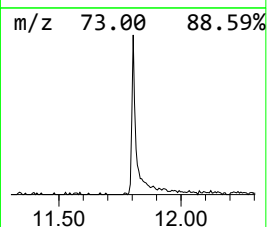
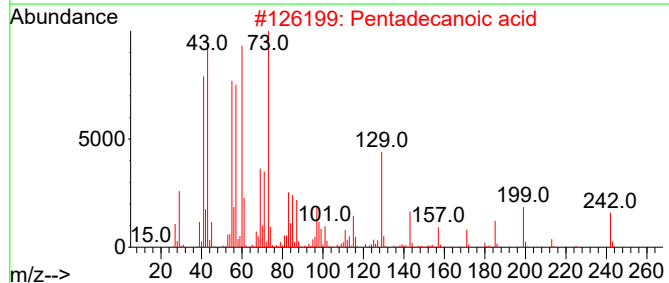
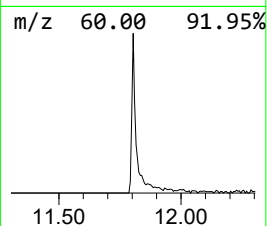
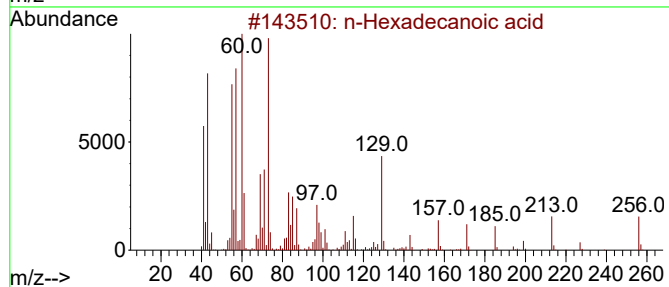
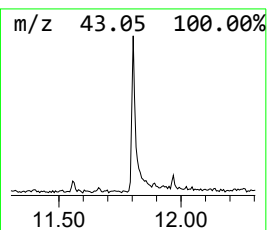
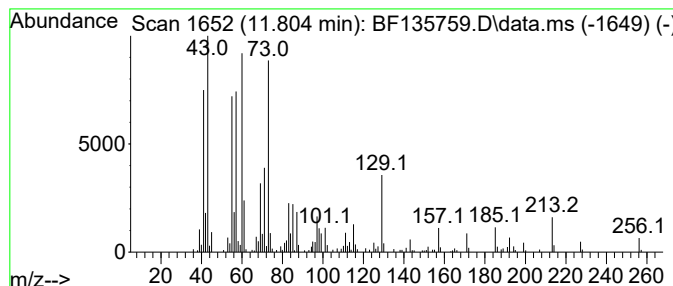
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	4.79 ng	224273	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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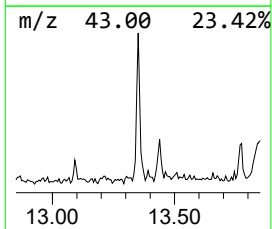
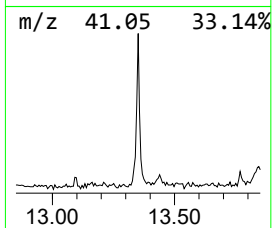
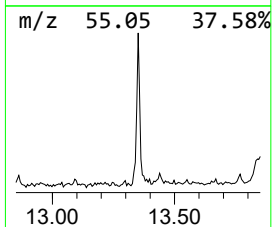
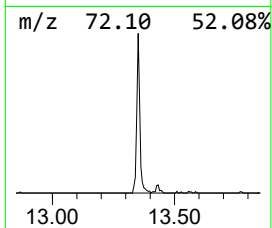
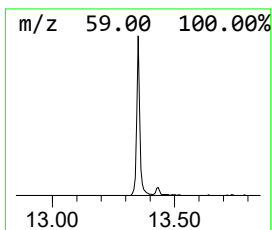
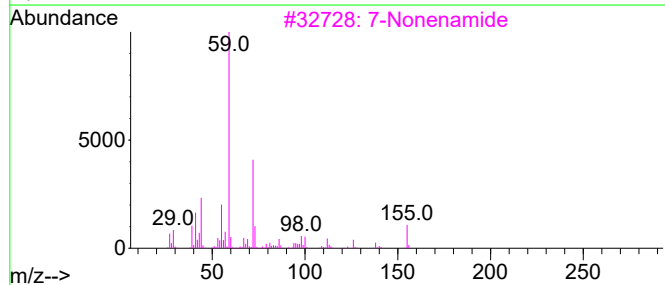
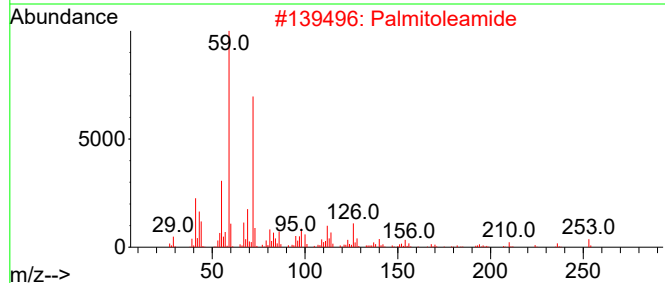
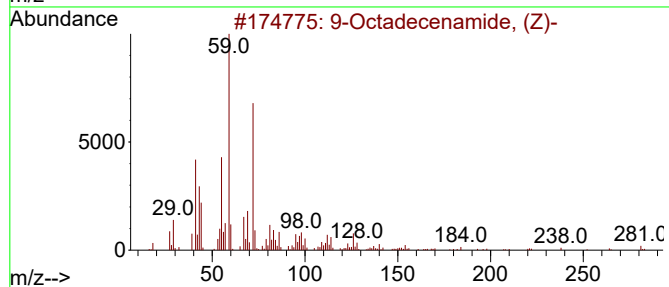
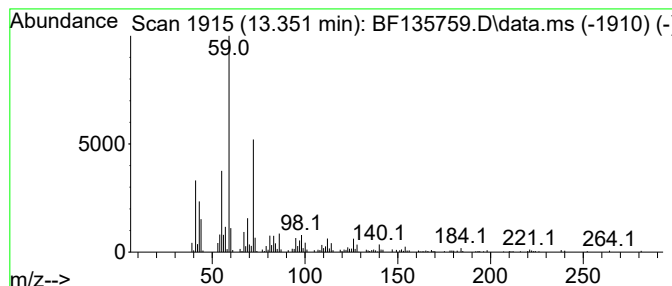
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.351	7.02 ng	208487	Chrysene-d12		13.933

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91	
2	Palmitoleamide	253	C16H31NO	106010-22-4	83	
3	7-Nonenamide	155	C9H17NO	090949-53-4	72	
4	Octanamide	143	C8H17NO	000629-01-6	53	
5	Nonanamide	157	C9H19NO	001120-07-6	53	



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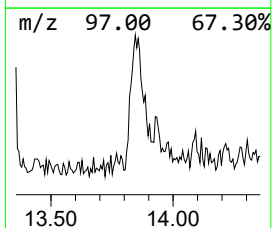
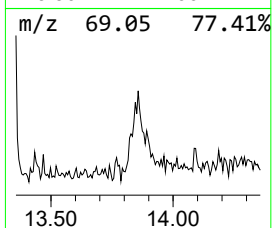
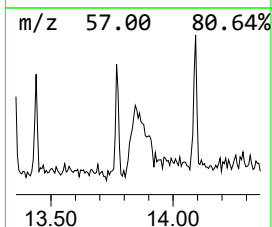
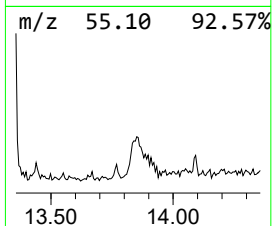
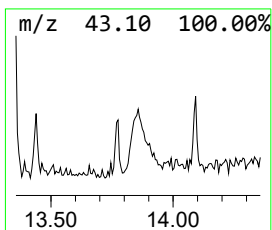
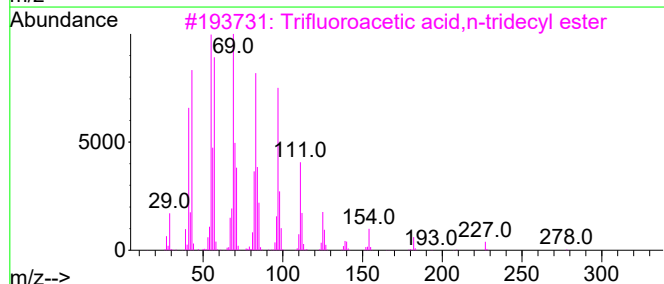
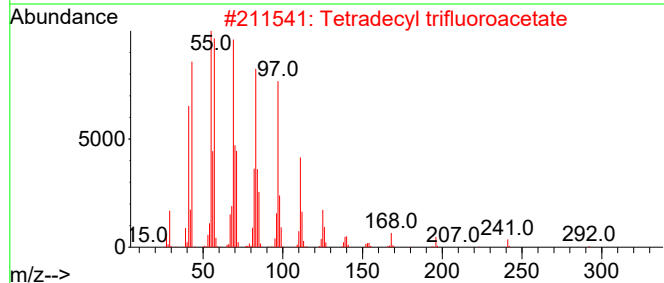
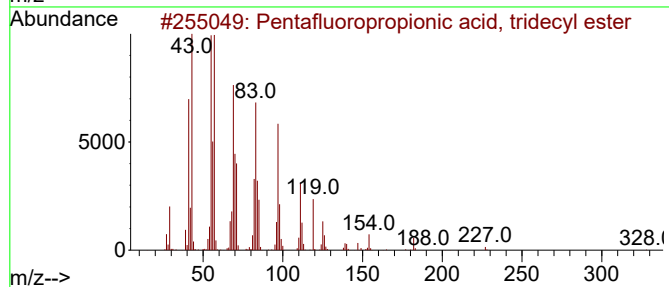
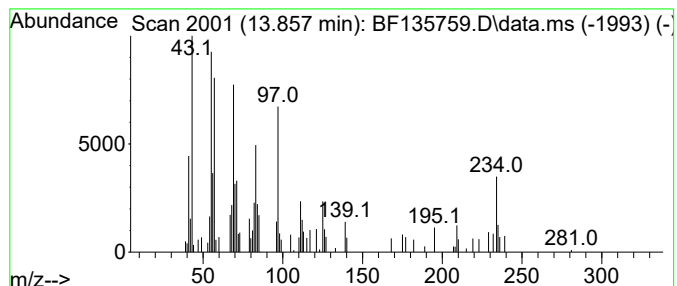
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.64 ng	78459	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tridecyl...	346	C16H27F5O2	959261-22-4	81
2			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	81
3			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	74
4			1-Tridecene	182	C13H26	002437-56-1	64
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135759.D
Acq On : 13 Oct 2023 18:39
Operator : CG\JU
Sample : 04844-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-603-COMP-07

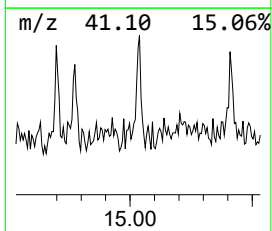
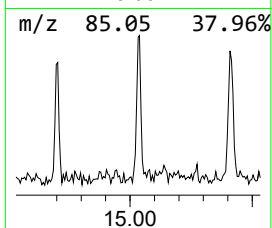
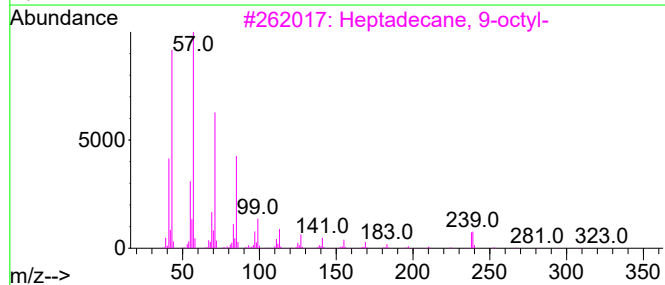
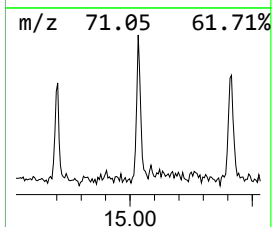
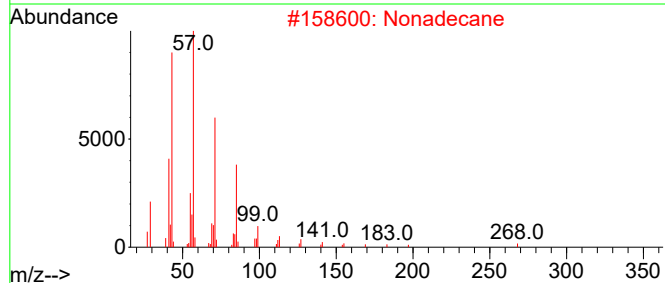
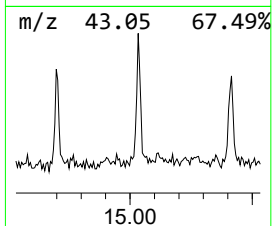
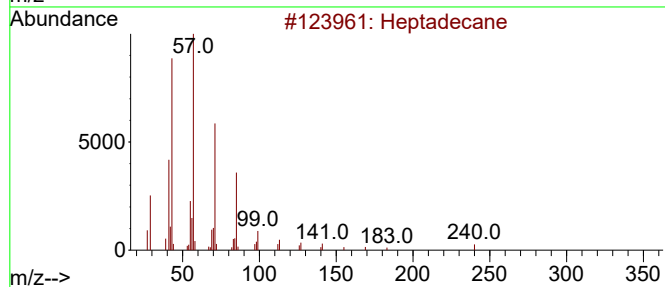
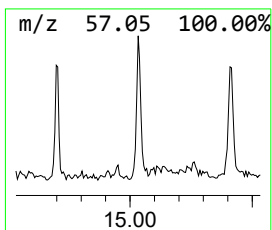
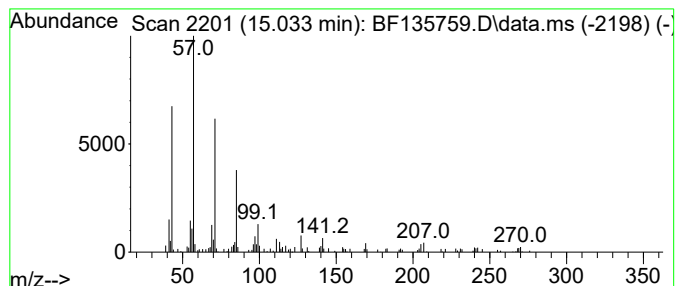
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	2.20 ng	79900	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	91
2			Nonadecane	268	C19H40	000629-92-5	87
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4			Decane, 2-methyl-	156	C11H24	006975-98-0	72
5			Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135759.D
Acq On : 13 Oct 2023 18:39
Operator : CG\JU
Sample : 04844-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-603-COMP-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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-...	4.969	3.4	ng	126015	1	6.734	734683	20.0
Tridecane	8.604	2.0	ng	90629	2	8.016	902819	20.0
n-Hexadecanoic ...	11.804	4.8	ng	224273	4	11.269	935664	20.0
9-Octadecenamid...	13.351	7.0	ng	208487	5	13.933	594026	20.0
Pentafluoroprop...	13.857	2.6	ng	78459	5	13.933	594026	20.0
Heptadecane	15.033	2.2	ng	79900	6	15.410	725606	20.0