

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
 Data File : BF125236.D
 Acq On : 26 Aug 2021 21:17
 Operator : JU/CG
 Sample : M3543-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125236.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	31	rVB	1903944	2599272	46.23%	5.889%
2	5.151	517	521	527	rVB	70498	86399	1.54%	0.196%
3	5.534	581	586	589	rBV	5176411	5409095	96.20%	12.255%
4	6.540	751	757	760	rBV	4905670	5238187	93.16%	11.868%
5	6.910	817	820	824	rBV	1411575	1186449	21.10%	2.688%
6	7.475	911	916	919	rBV	3686363	3499111	62.23%	7.928%
7	8.092	1018	1021	1032	rBV	157135	312845	5.56%	0.709%
8	8.192	1035	1038	1042	rBV	1639889	1457413	25.92%	3.302%
9	9.269	1216	1221	1224	rBV	6343477	5622559	100.00%	12.739%
10	9.945	1333	1336	1340	rBV	1644933	1502469	26.72%	3.404%
11	10.733	1466	1470	1474	rBV	3339465	3302241	58.73%	7.482%
12	11.433	1585	1589	1592	rBV	1640707	1413068	25.13%	3.202%
13	11.457	1592	1593	1596	rVB	288095	171647	3.05%	0.389%
14	11.951	1672	1677	1682	rBV2	600945	637969	11.35%	1.445%
15	12.045	1690	1693	1696	rBV2	63879	67969	1.21%	0.154%
16	12.645	1792	1795	1800	rBV	530113	520107	9.25%	1.178%
17	12.739	1808	1811	1816	rBV2	280049	284574	5.06%	0.645%
18	12.874	1828	1834	1839	rBV	464454	508883	9.05%	1.153%
19	13.021	1855	1859	1862	rBV	5287640	4509666	80.21%	10.217%
20	13.092	1867	1871	1876	rBV3	47723	75075	1.34%	0.170%
21	13.204	1888	1890	1894	rVB	79397	63852	1.14%	0.145%
22	13.310	1903	1908	1910	rBV2	61071	65510	1.17%	0.148%
23	13.551	1946	1949	1952	rBV	65231	61756	1.10%	0.140%
24	13.710	1973	1976	1982	rVB	69540	71579	1.27%	0.162%
25	13.916	2008	2011	2013	rBV2	82614	75451	1.34%	0.171%
26	13.974	2017	2021	2022	rBV3	69565	93678	1.67%	0.212%
27	14.051	2030	2034	2035	rBV	306255	300419	5.34%	0.681%
28	14.074	2035	2038	2041	rVV	1454910	1469776	26.14%	3.330%
29	14.098	2041	2042	2045	rVB	343345	213039	3.79%	0.483%
30	14.539	2114	2117	2119	rBV2	56912	65812	1.17%	0.149%
31	14.704	2142	2145	2150	rBV2	73198	103150	1.83%	0.234%
32	15.004	2193	2196	2198	rVB	104401	100307	1.78%	0.227%
33	15.127	2213	2217	2220	rBV	300308	438037	7.79%	0.992%
34	15.204	2227	2230	2233	rVB2	101079	117022	2.08%	0.265%
35	15.439	2267	2270	2277	rVB	196617	245934	4.37%	0.557%
36	15.504	2277	2281	2287	rBV	220700	273258	4.86%	0.619%

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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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.574	2287	2293	2296	rBV	1044465	1395788	24.82%	3.162%
38	16.045	2370	2373	2379	rVB	109044	160327	2.85%	0.363%
39	17.074	2544	2548	2557	rVB2	101667	206559	3.67%	0.468%
40	17.527	2621	2625	2634	rVB	93608	211193	3.76%	0.478%

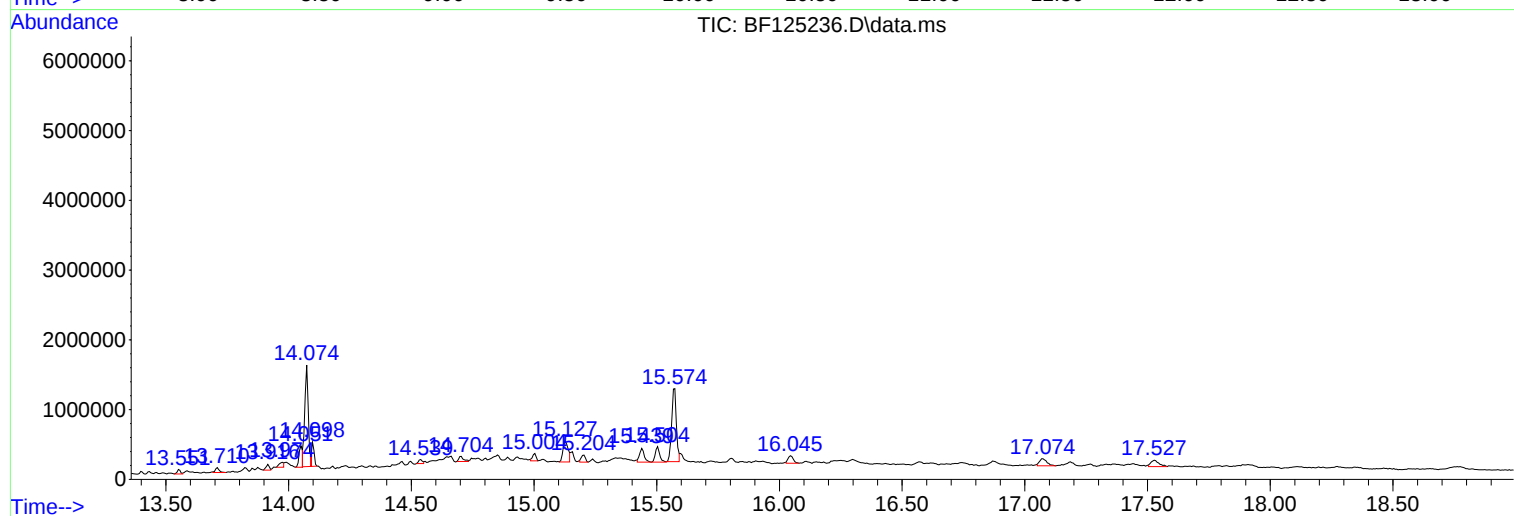
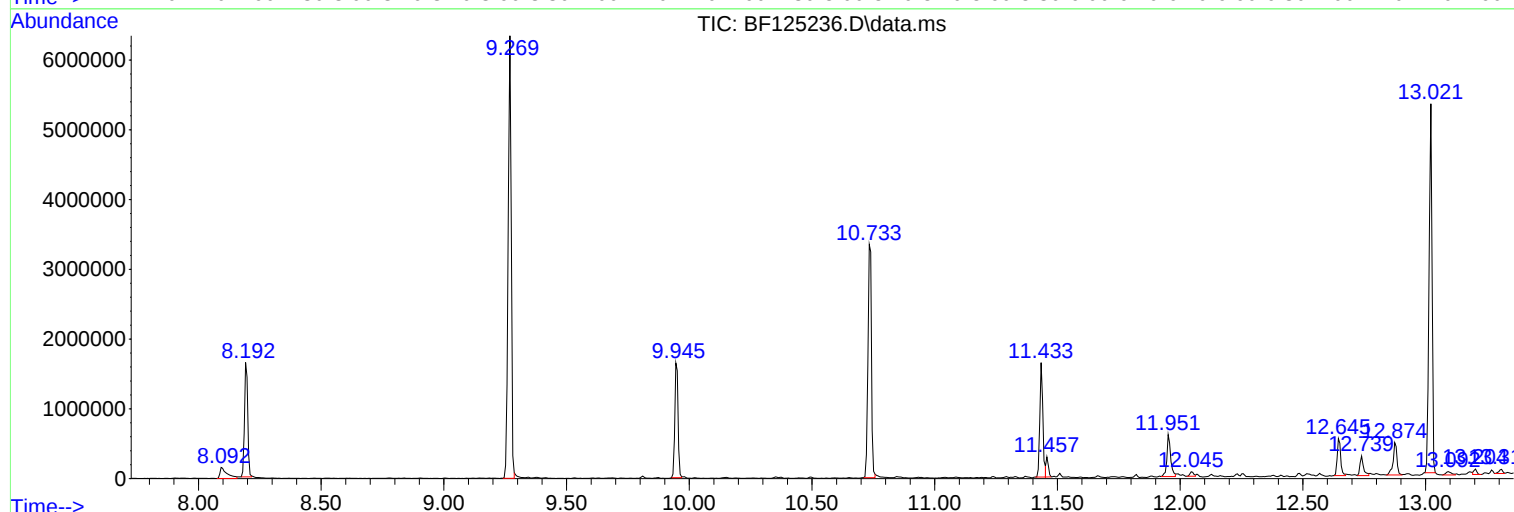
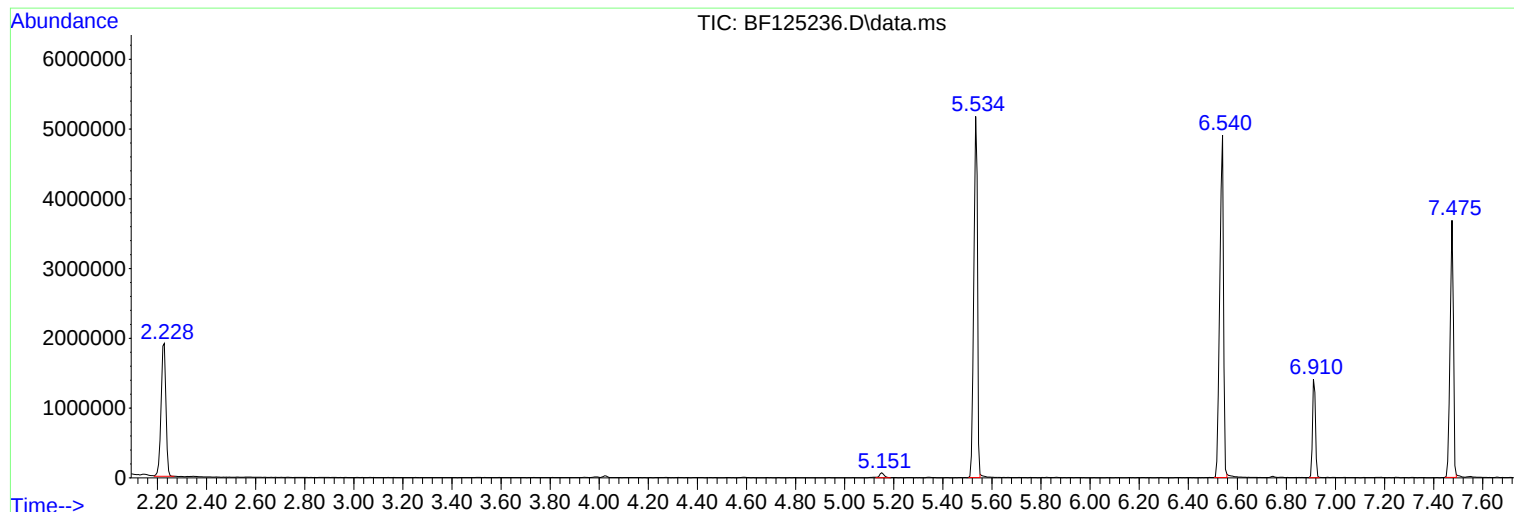
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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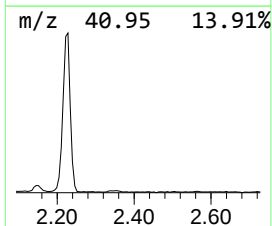
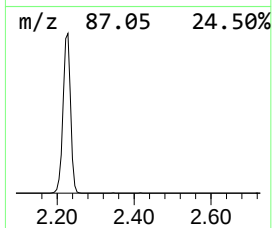
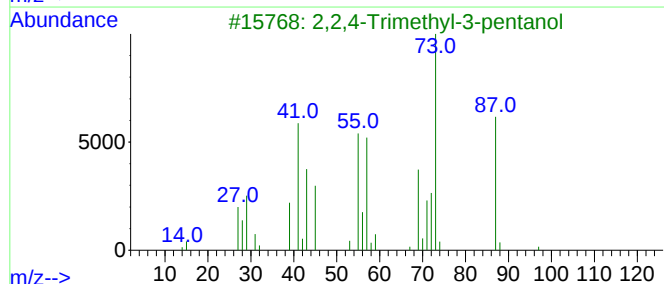
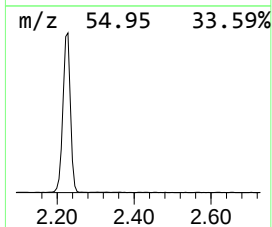
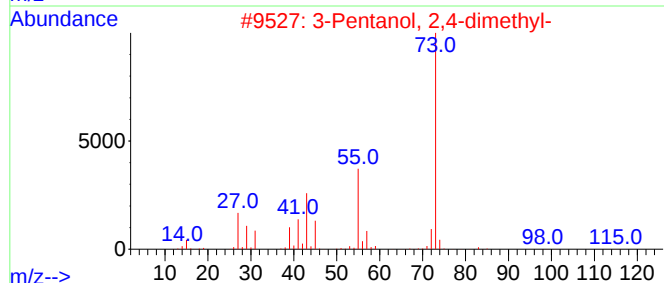
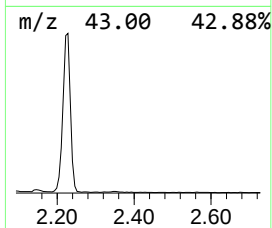
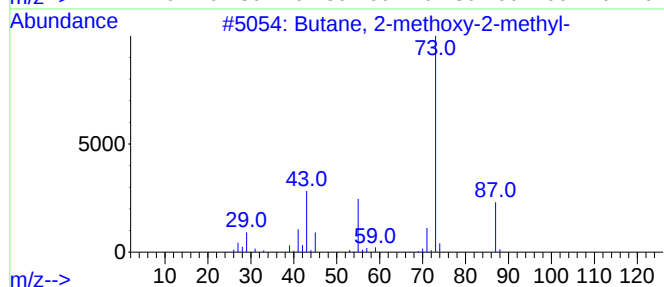
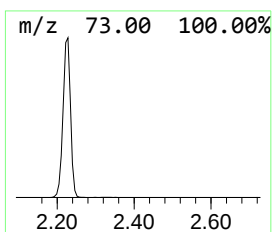
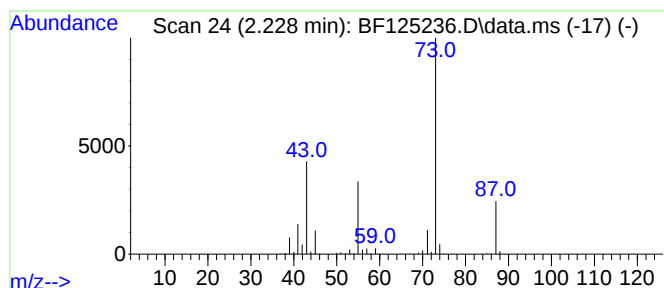
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	43.82 ng	2599270	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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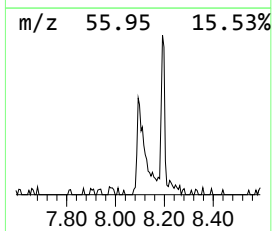
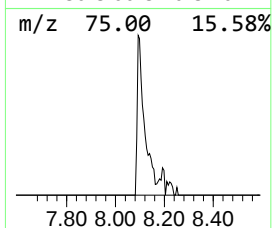
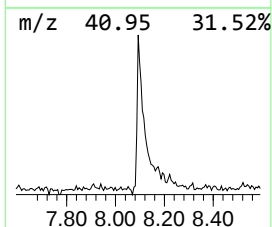
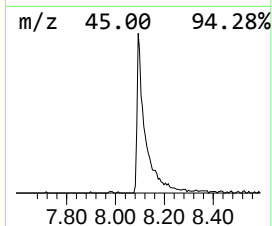
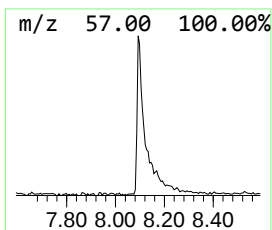
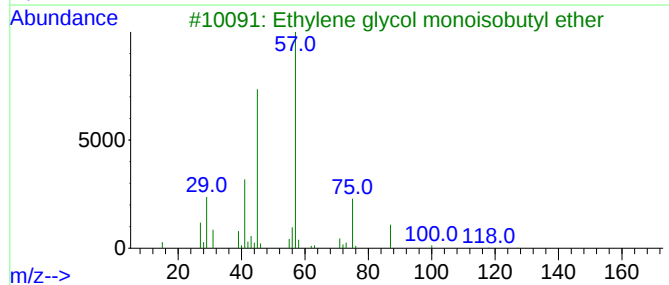
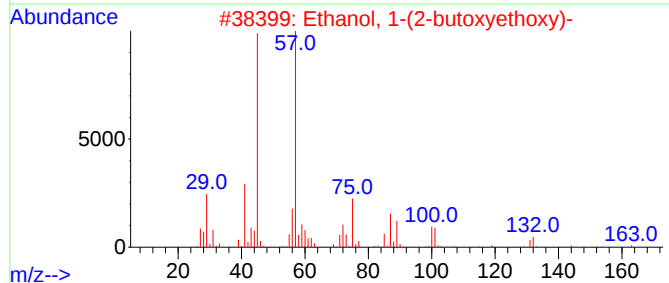
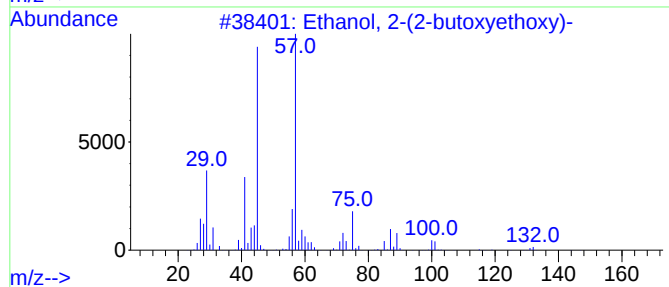
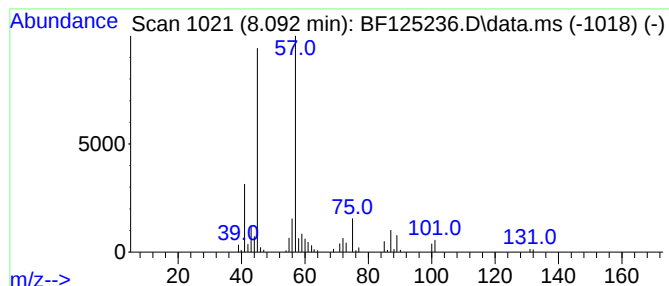
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	4.29 ng	312845	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	53



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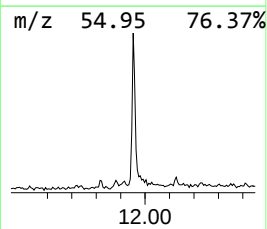
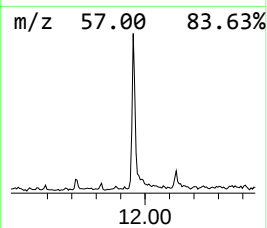
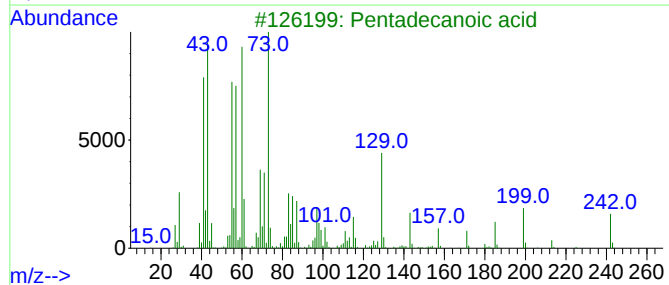
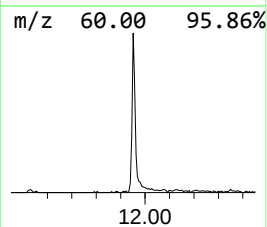
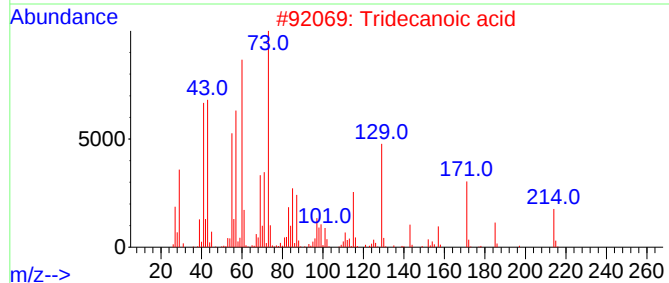
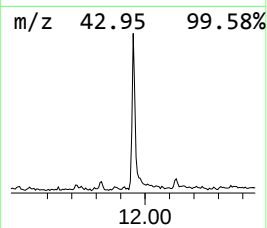
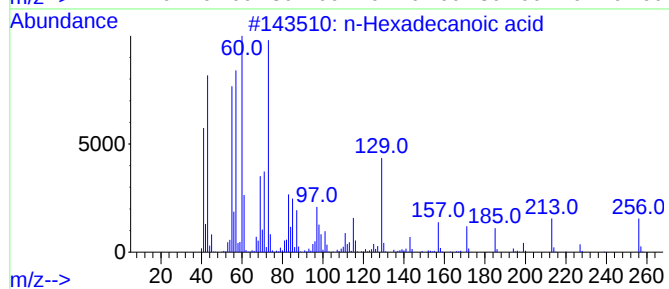
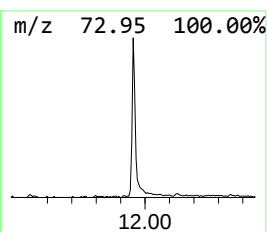
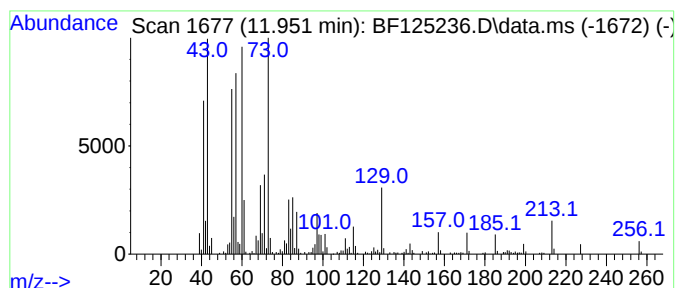
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.951	9.03 ng	637969	Phenanthrene-d10		11.433	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
5	Undecanoic acid		186	C11H22O2	000112-37-8	72



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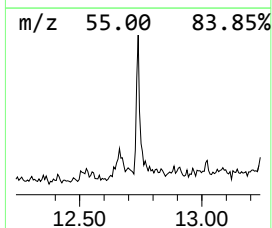
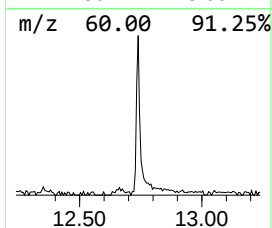
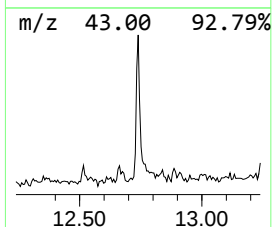
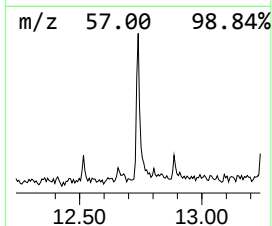
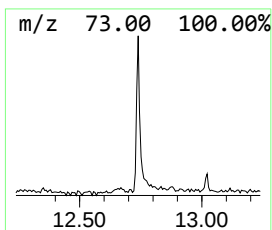
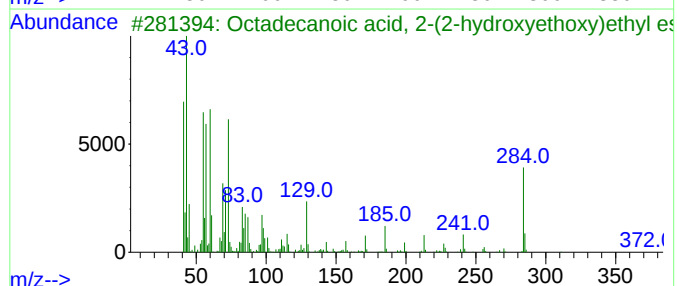
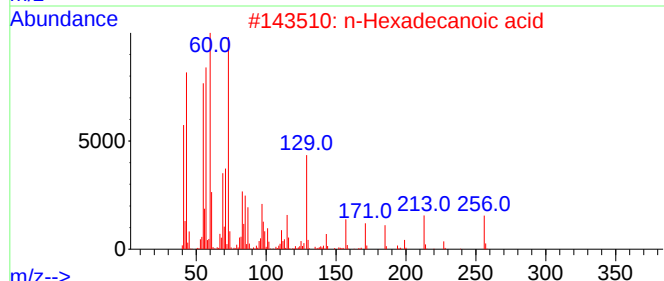
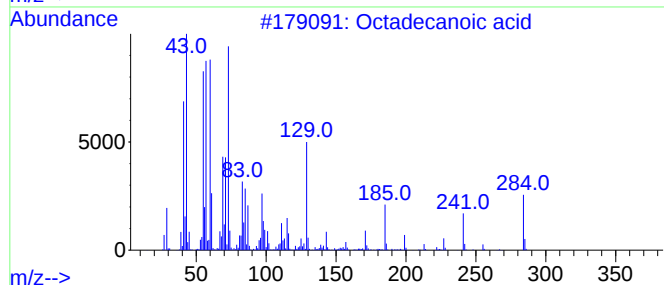
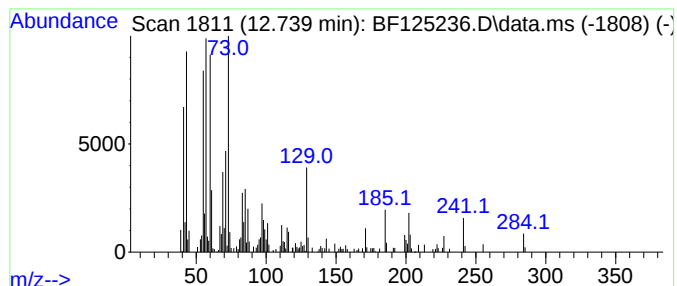
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	4.03 ng	284574	Phenanthrene-d10	11.433

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	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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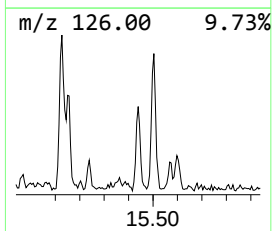
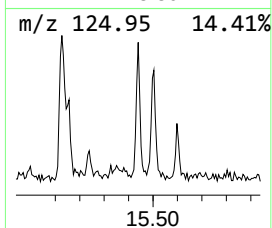
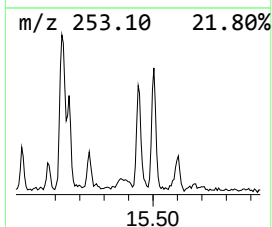
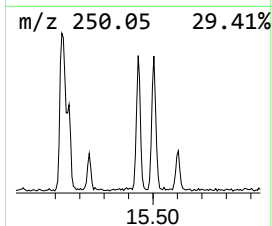
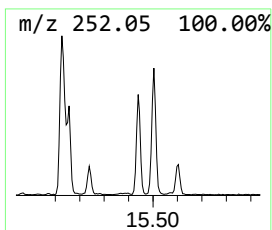
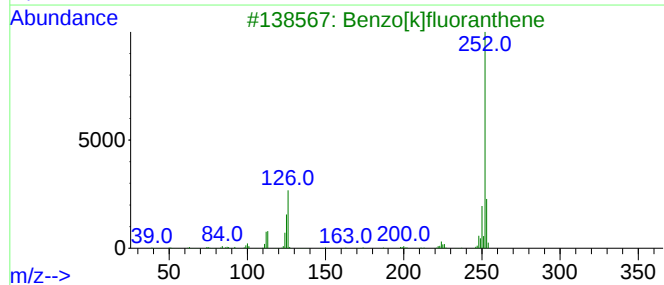
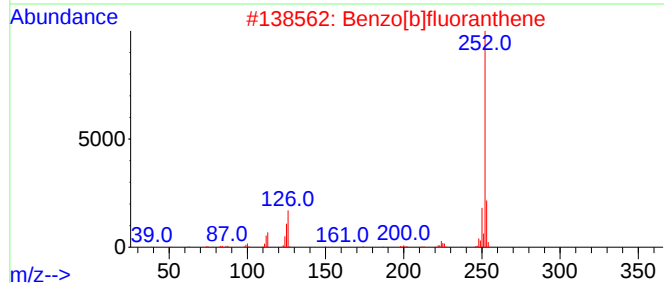
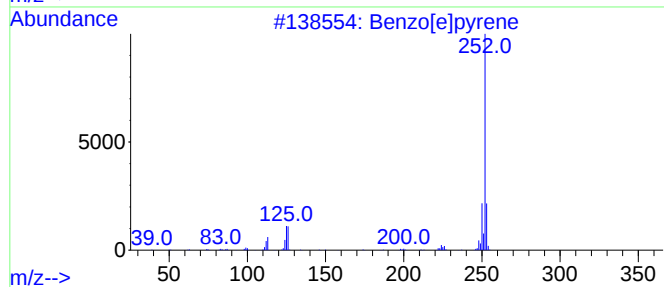
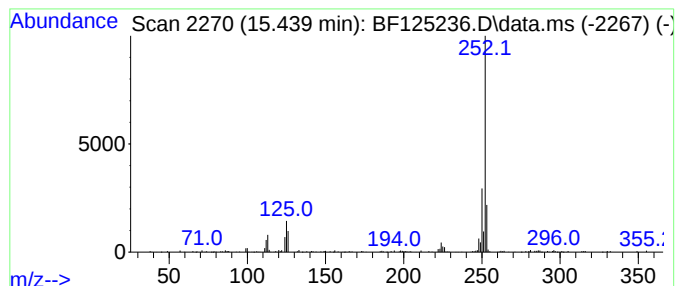
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	3.52 ng	245934	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125236.D
Acq On : 26 Aug 2021 21:17
Operator : JU/CG
Sample : M3543-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP

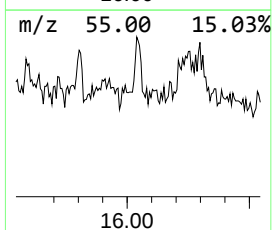
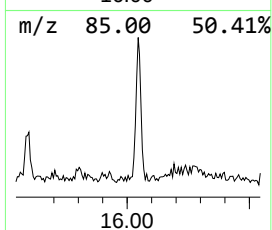
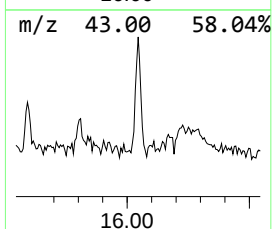
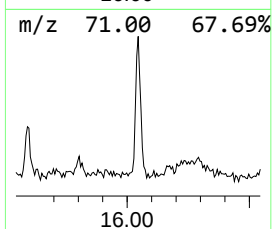
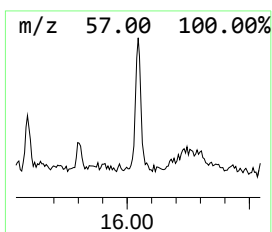
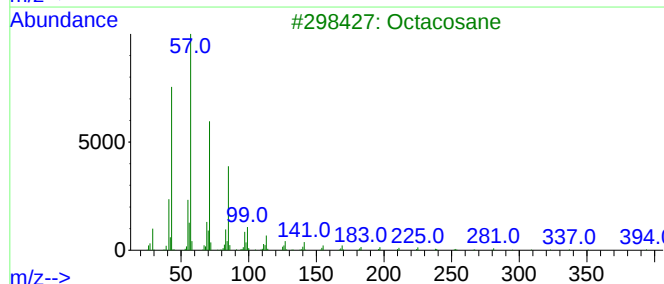
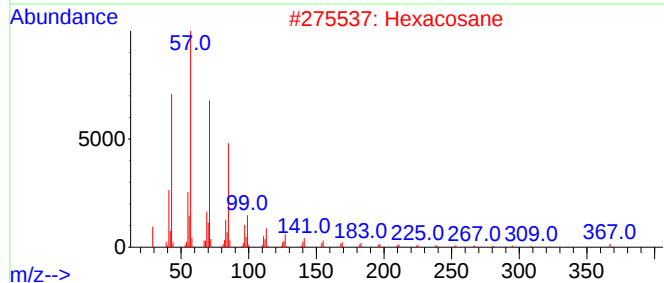
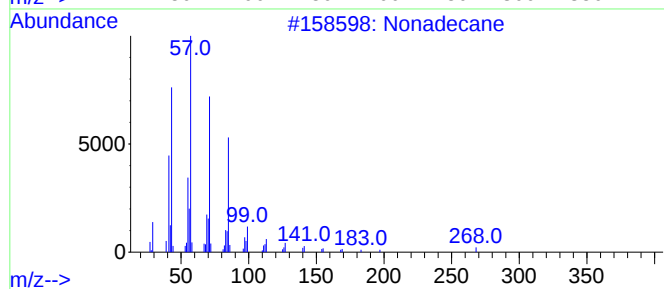
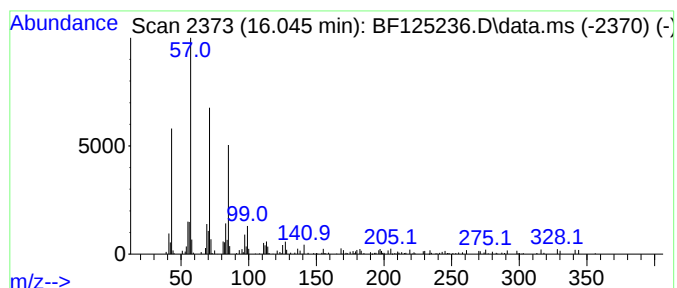
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	2.30 ng	160327	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			Octacosane	394	C28H58	000630-02-4	83
4			Tetracosane	338	C24H50	000646-31-1	83
5			Tetradecane	198	C14H30	000629-59-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125236.D
Acq On : 26 Aug 2021 21:17
Operator : JU/CG
Sample : M3543-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	43.8	ng	2599270	1	6.910	1186450	20.0
Ethanol, 2-(2-b...	8.092	4.3	ng	312845	2	8.192	1457410	20.0
n-Hexadecanoic ...	11.951	9.0	ng	637969	4	11.433	1413070	20.0
Octadecanoic acid	12.739	4.0	ng	284574	4	11.433	1413070	20.0
Benzo[e]pyrene	15.439	3.5	ng	245934	6	15.574	1395790	20.0
Nonadecane	16.045	2.3	ng	160327	6	15.574	1395790	20.0