

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125933.D
 Acq On : 26 Oct 2021 14:18
 Operator : JU/CG
 Sample : M4308-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	5	12	18	rVB	2140876	2793518	71.32%	8.311%
2	3.352	211	215	228	rBV	20241	49878	1.27%	0.148%
3	5.087	502	510	518	rVB	93053	127617	3.26%	0.380%
4	5.481	571	577	580	rBV	4108732	3906059	99.72%	11.621%
5	6.487	742	748	751	rBV	3750954	3916847	100.00%	11.653%
6	6.863	809	812	816	rBV	1140346	960626	24.53%	2.858%
7	7.428	903	908	911	rBV	2571861	2482249	63.37%	7.385%
8	8.051	1010	1014	1017	rBV	1018903	736364	18.80%	2.191%
9	8.151	1026	1031	1034	rBV	1405364	1272899	32.50%	3.787%
10	9.228	1209	1214	1217	rBV	3903693	3521477	89.91%	10.477%
11	9.345	1231	1234	1237	rVB	114316	92516	2.36%	0.275%
12	9.904	1325	1329	1332	rBV	1675155	1383905	35.33%	4.117%
13	10.686	1458	1462	1465	rBV	3010691	2633126	67.23%	7.834%
14	11.386	1577	1581	1583	rBV	1853059	1492797	38.11%	4.441%
15	11.410	1583	1585	1588	rVV	247290	185527	4.74%	0.552%
16	11.457	1588	1593	1596	rVB3	111054	103821	2.65%	0.309%
17	11.786	1646	1649	1653	rVB	72891	57820	1.48%	0.172%
18	11.916	1668	1671	1675	rBV2	208822	168529	4.30%	0.501%
19	11.998	1681	1685	1687	rBV	39292	39943	1.02%	0.119%
20	12.492	1767	1769	1772	rVB	142480	117584	3.00%	0.350%
21	12.598	1781	1787	1790	rBV	227367	245635	6.27%	0.731%
22	12.698	1801	1804	1811	rBV5	41577	59792	1.53%	0.178%
23	12.822	1819	1825	1829	rBV2	181601	207038	5.29%	0.616%
24	12.974	1847	1851	1854	rBV	3917052	3766284	96.16%	11.205%
25	13.186	1884	1887	1890	rBV	140347	116963	2.99%	0.348%
26	13.427	1925	1928	1931	rBV	91165	67823	1.73%	0.202%
27	13.522	1940	1944	1948	rBV2	43634	51446	1.31%	0.153%
28	13.874	2000	2004	2013	rBV2	415495	416549	10.63%	1.239%
29	14.021	2024	2029	2032	rBV	1354421	1357892	34.67%	4.040%
30	14.045	2032	2033	2038	rVB	78690	64860	1.66%	0.193%
31	14.510	2109	2112	2118	rBV4	45351	56968	1.45%	0.169%
32	14.898	2175	2178	2182	rBV	64138	64508	1.65%	0.192%
33	15.063	2203	2206	2216	rVB3	38227	77142	1.97%	0.230%
34	15.168	2221	2224	2230	rVB4	29644	41911	1.07%	0.125%
35	15.421	2264	2267	2274	rBV2	34460	48645	1.24%	0.145%
36	15.492	2274	2279	2284	rBV	758127	925731	23.63%	2.754%

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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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

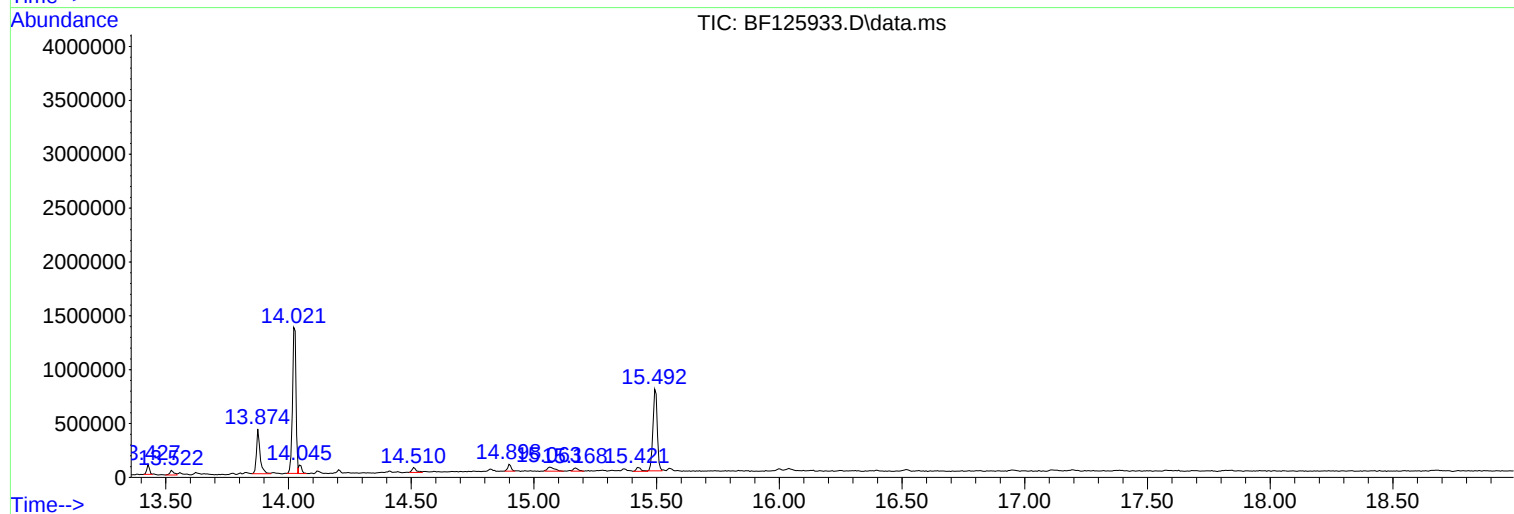
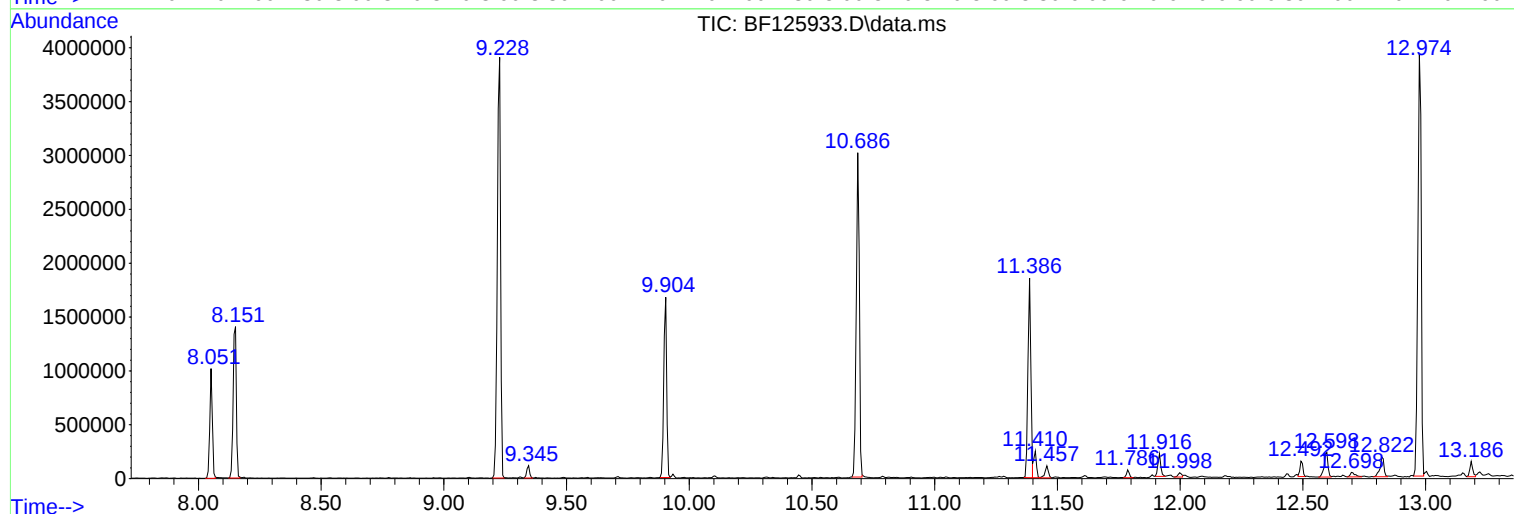
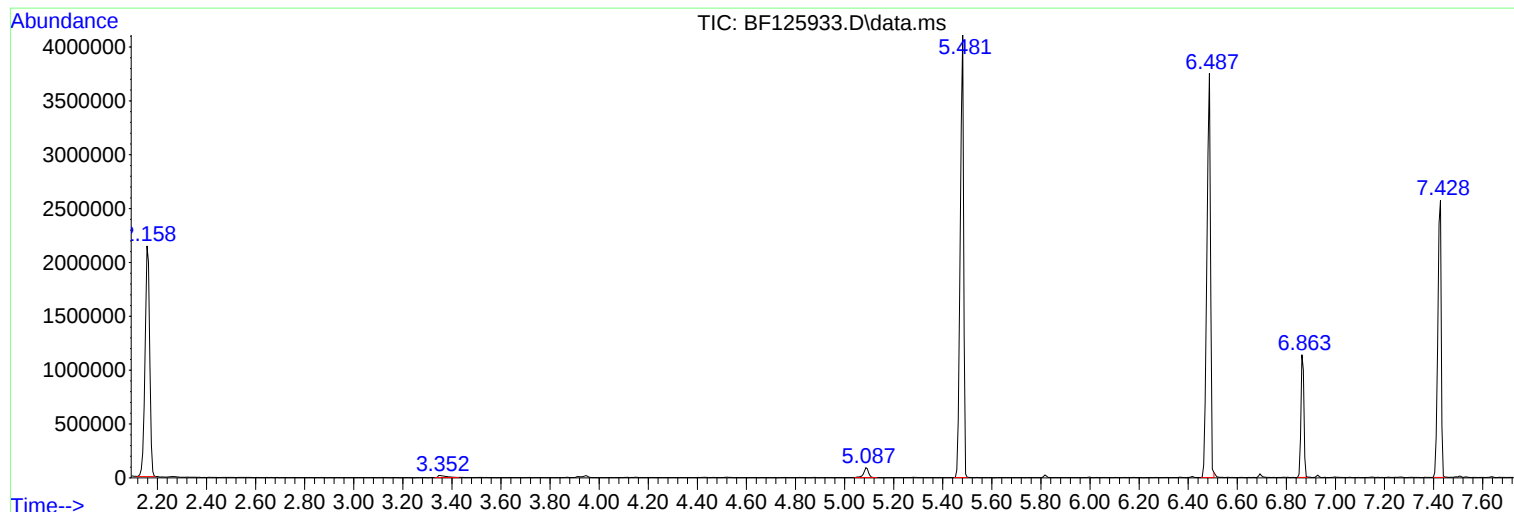
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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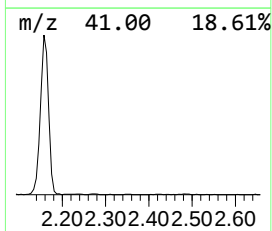
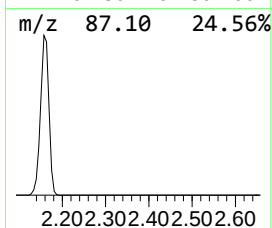
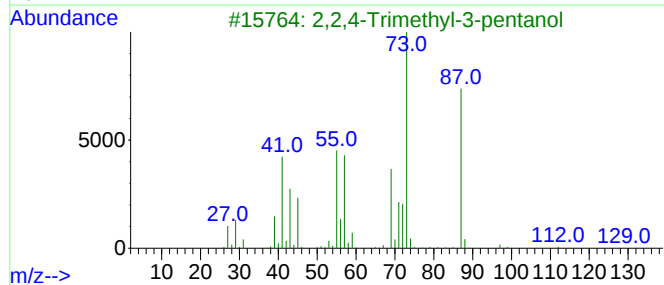
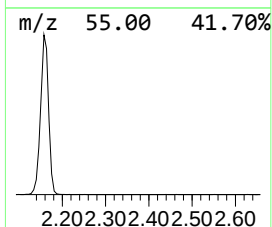
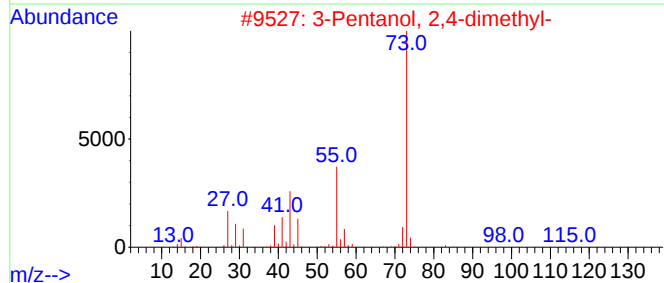
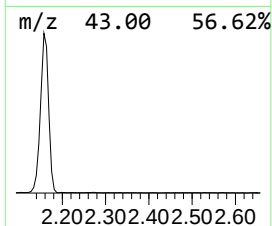
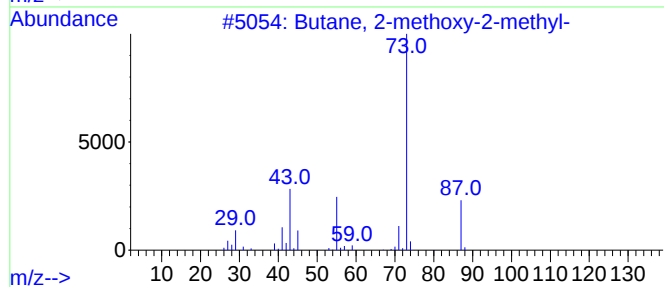
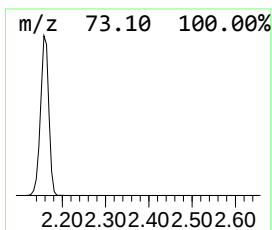
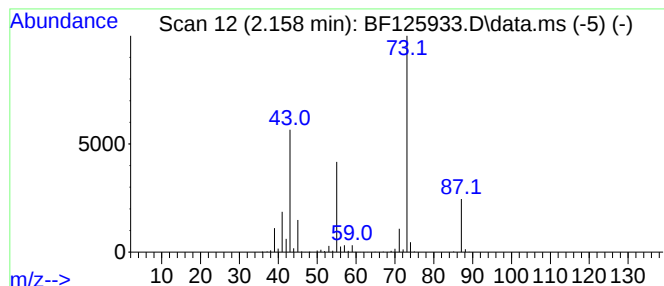
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.158	58.16 ng	2793520	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	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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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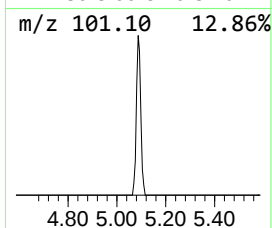
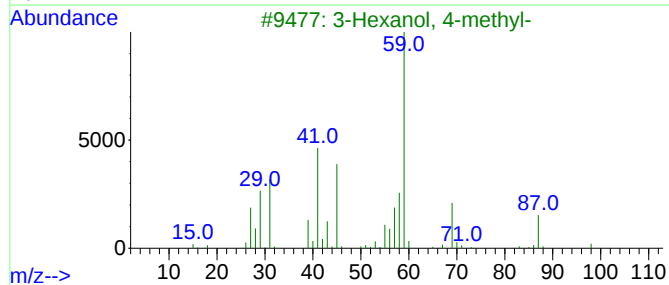
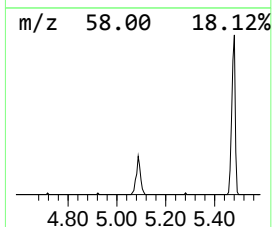
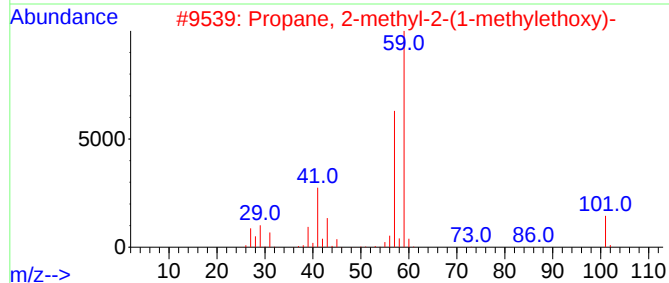
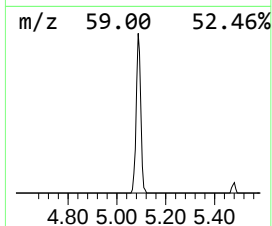
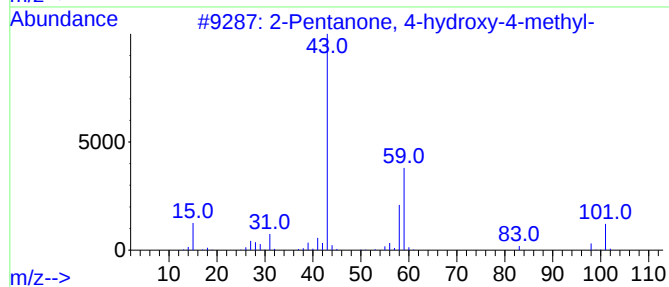
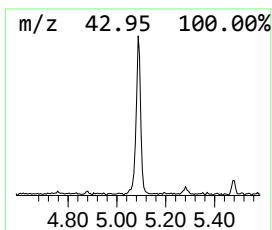
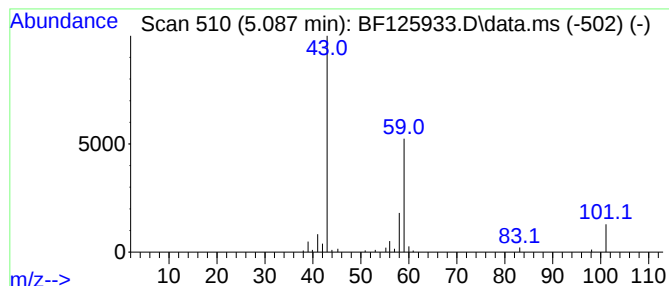
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.66 ng	127617	1,4-Dichlorobenzene-d4	6.863

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-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	3-Pentanol	88	C5H12O	000584-02-1	25		



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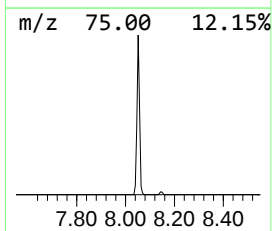
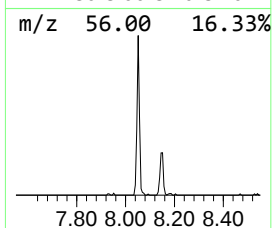
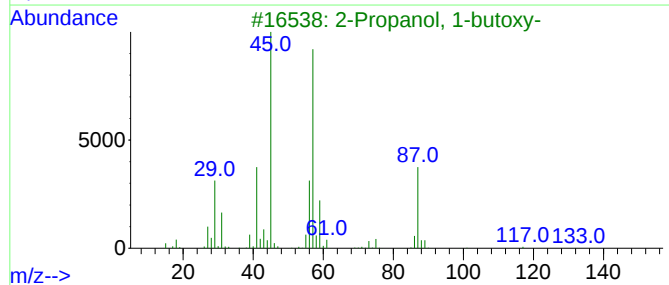
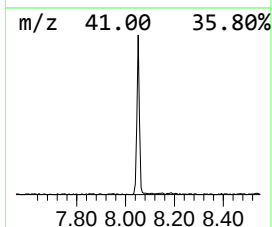
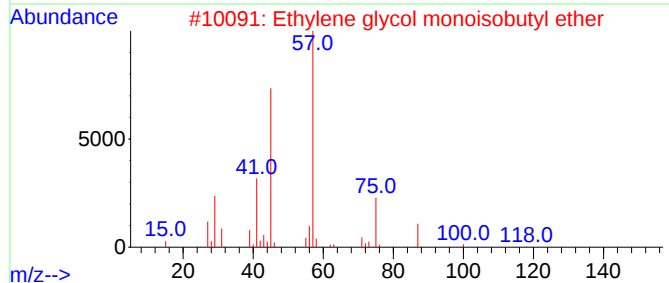
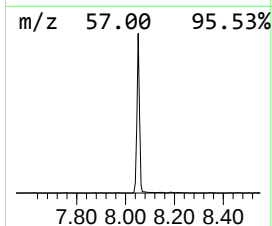
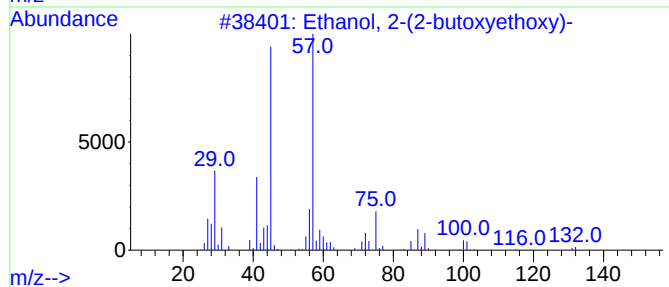
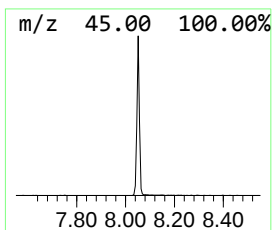
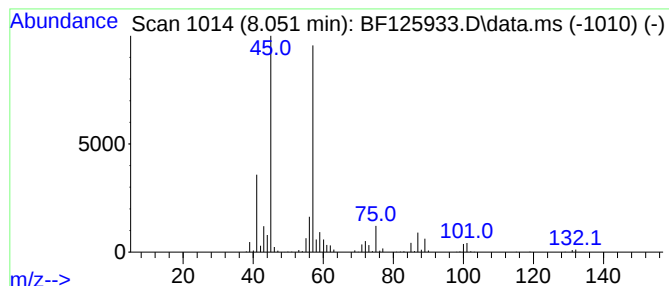
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	11.57 ng	736364	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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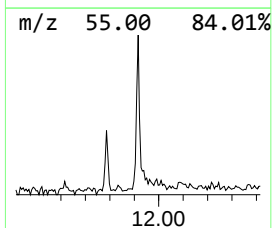
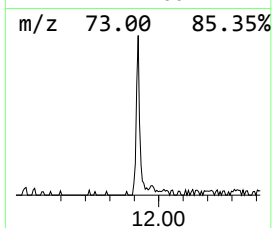
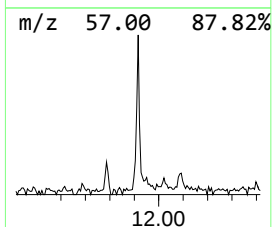
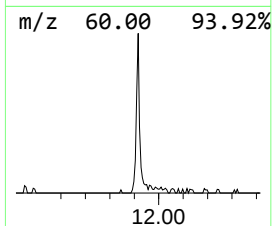
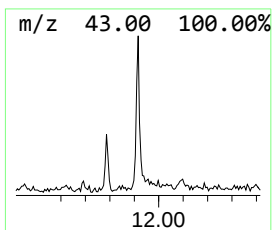
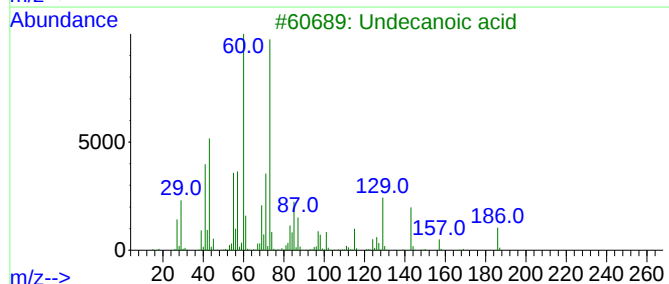
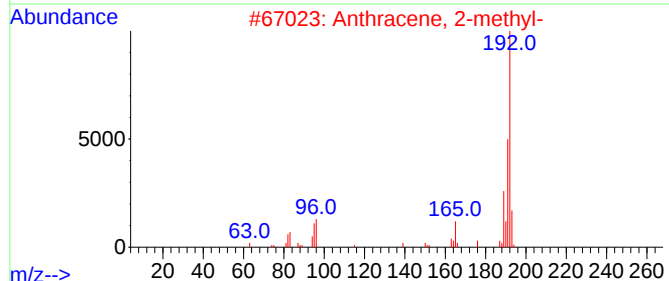
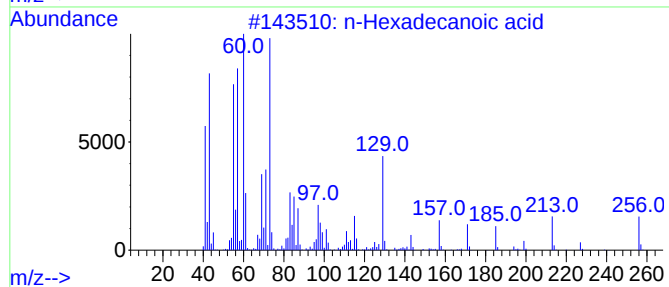
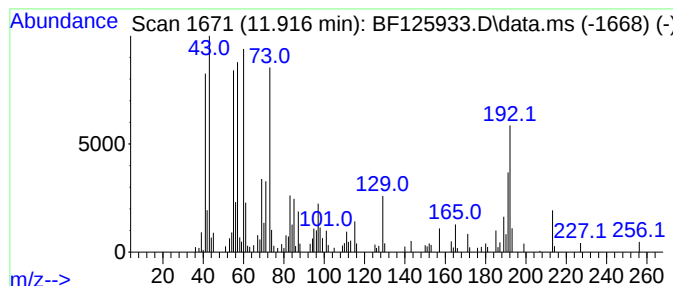
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.26 ng	168529	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	80
3			Undecanoic acid	186	C11H22O2	000112-37-8	55
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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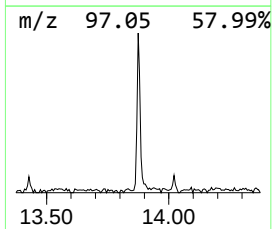
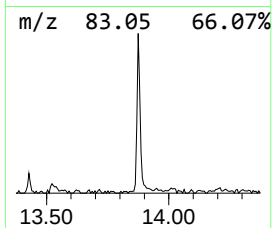
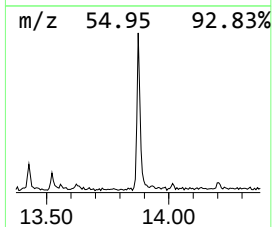
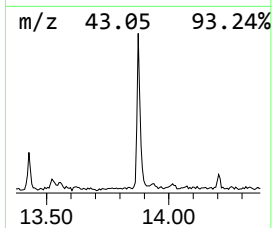
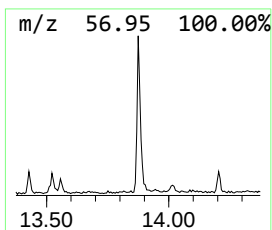
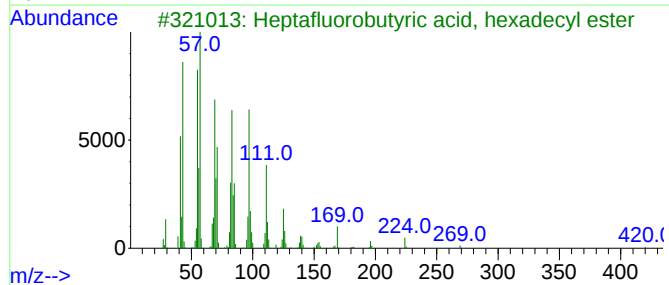
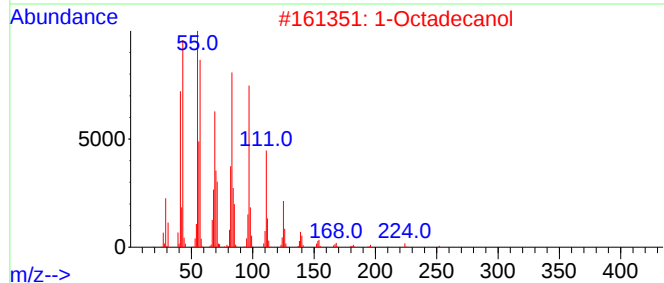
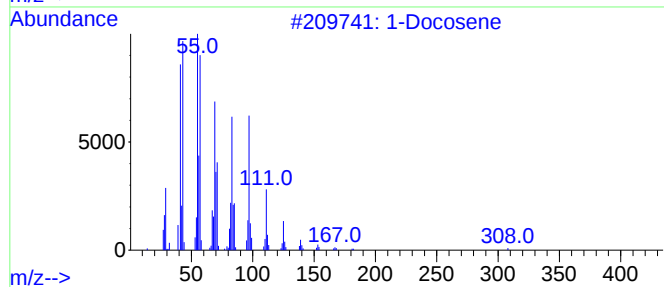
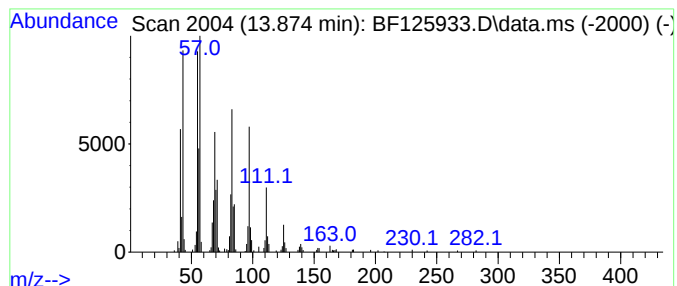
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.14 ng	416549	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	95
2	1-Octadecanol		270	C18H38O	000112-92-5	91
3	Heptafluorobutyric acid, hexadec...		438	C20H33F7O2	006385-15-5	90
4	1-Heneicosanol		312	C21H44O	015594-90-8	90
5	Behenic alcohol		326	C22H46O	000661-19-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125933.D
Acq On : 26 Oct 2021 14:18
Operator : JU/CG
Sample : M4308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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...	2.158	58.2	ng	2793520	1	6.863	960626	20.0
2-Pentanone, 4-...	5.087	2.7	ng	127617	1	6.863	960626	20.0
Ethanol, 2-(2-b...	8.051	11.6	ng	736364	2	8.151	1272900	20.0
n-Hexadecanoic ...	11.916	2.3	ng	168529	4	11.386	1492800	20.0
1-Docosene	13.874	6.1	ng	416549	5	14.027	1357890	20.0