

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125941.D
 Acq On : 26 Oct 2021 19:01
 Operator : JU/CG
 Sample : M4340-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TH-ES

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: BF125941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	6	12	18	rVB	2588419	3344312	77.14%	9.324%
2	3.345	212	214	224	rBV	26912	58991	1.36%	0.164%
3	5.092	508	511	515	rVB	45801	52829	1.22%	0.147%
4	5.481	572	577	580	rBV	4354142	4231631	97.61%	11.798%
5	6.486	742	748	751	rBV	4046192	4335273	100.00%	12.087%
6	6.869	809	813	816	rBV	1280600	1118356	25.80%	3.118%
7	7.428	903	908	911	rBV	2925621	2859475	65.96%	7.972%
8	8.051	1010	1014	1017	rBV	1591035	1243674	28.69%	3.467%
9	8.145	1026	1030	1034	rBV	1597895	1469513	33.90%	4.097%
10	9.227	1209	1214	1217	rBV	4765212	4251194	98.06%	11.852%
11	9.904	1325	1329	1332	rVB	1846570	1581129	36.47%	4.408%
12	10.310	1395	1398	1406	rBV2	62912	74370	1.72%	0.207%
13	10.686	1458	1462	1465	rBV	3301415	2864051	66.06%	7.985%
14	11.386	1577	1581	1584	rBV	1982301	1613496	37.22%	4.498%
15	11.786	1646	1649	1653	rVB	104478	79774	1.84%	0.222%
16	11.915	1667	1671	1682	rVB2	250549	243170	5.61%	0.678%
17	12.592	1782	1786	1789	rBV	110078	108193	2.50%	0.302%
18	12.698	1801	1804	1811	rBV4	69398	82535	1.90%	0.230%
19	12.821	1823	1825	1828	rVB	94340	79835	1.84%	0.223%
20	12.974	1847	1851	1854	rBV	4044806	3534775	81.54%	9.855%
21	13.874	2000	2004	2013	rBV	306806	312349	7.20%	0.871%
22	14.021	2024	2029	2032	rBV	1105089	999939	23.07%	2.788%
23	14.509	2108	2112	2114	rBV4	49932	52871	1.22%	0.147%
24	14.898	2174	2178	2182	rBV	151568	144040	3.32%	0.402%
25	15.062	2201	2206	2209	rBV3	28364	49137	1.13%	0.137%
26	15.162	2220	2223	2231	rVB7	30287	51152	1.18%	0.143%
27	15.492	2274	2279	2286	rBV	823968	972219	22.43%	2.710%
28	16.033	2367	2371	2376	rVB7	38169	60376	1.39%	0.168%

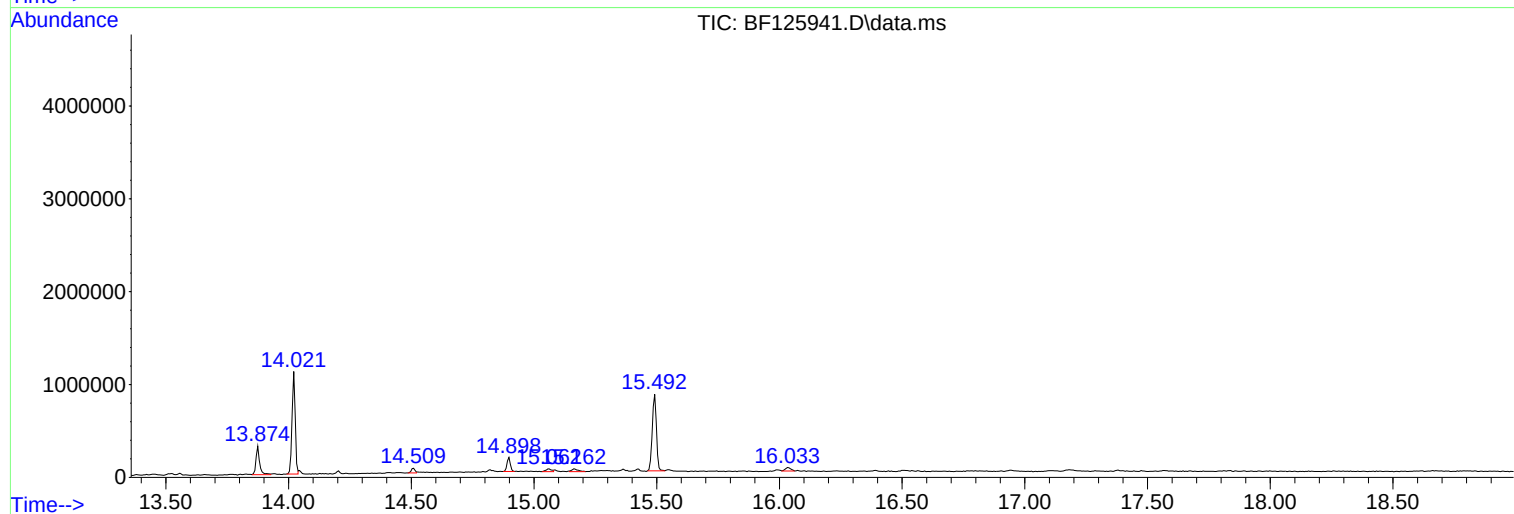
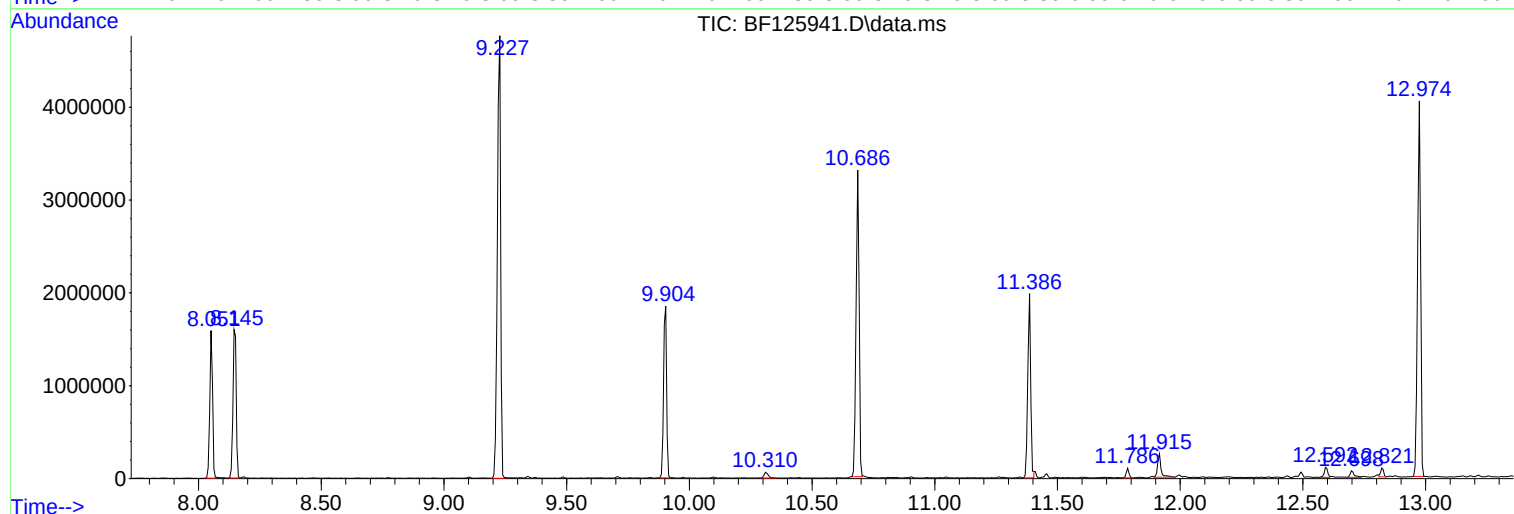
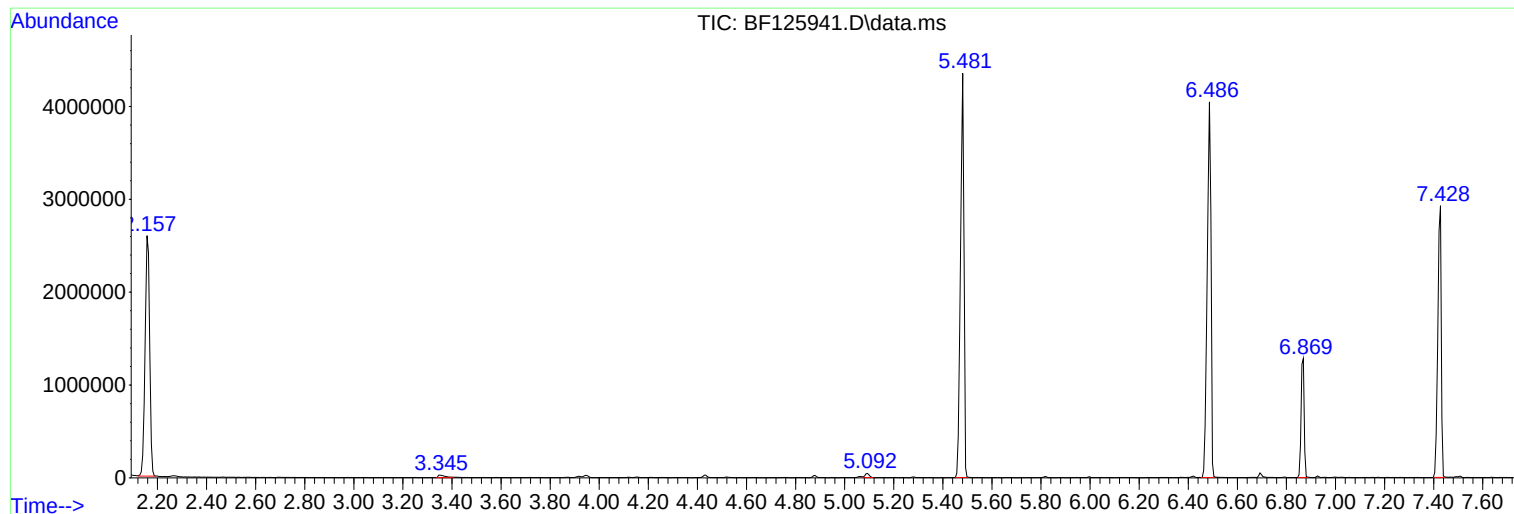
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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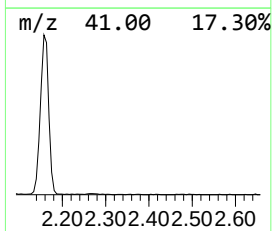
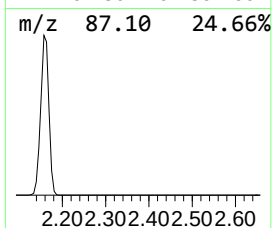
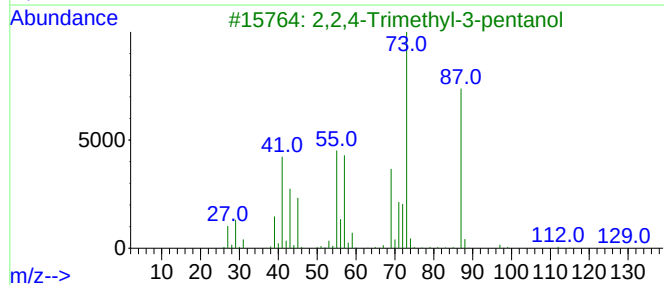
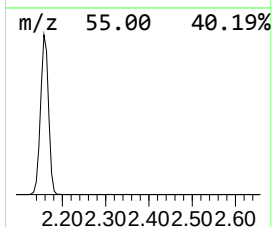
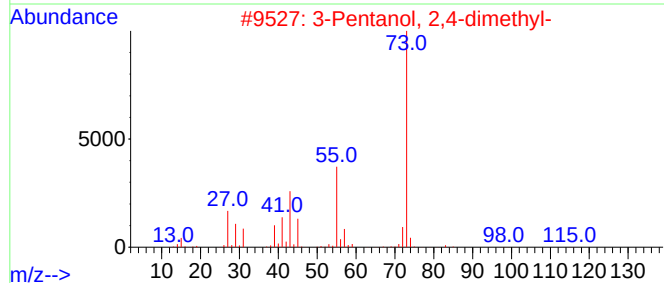
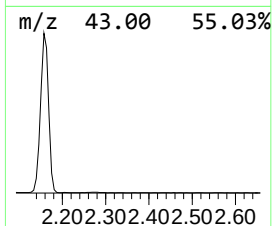
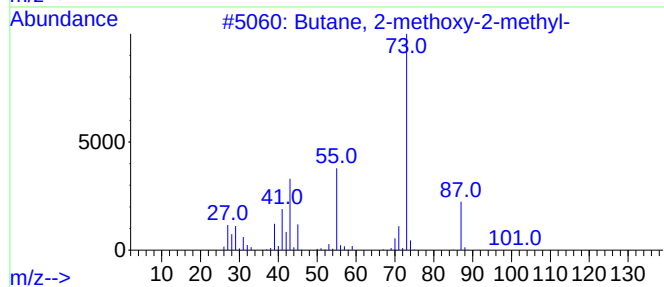
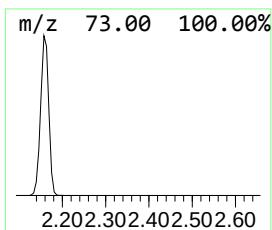
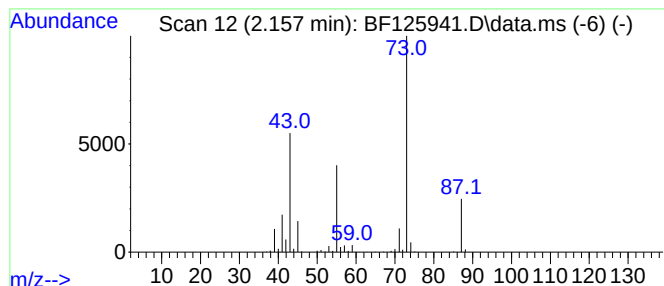
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.157	59.81 ng	3344310	1,4-Dichlorobenzene-d4	6.869

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



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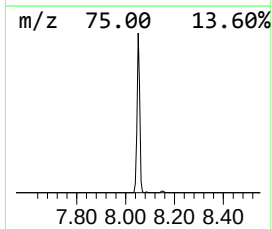
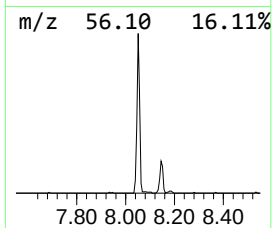
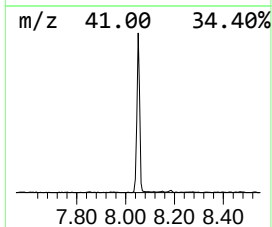
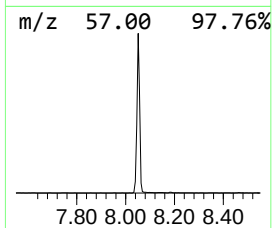
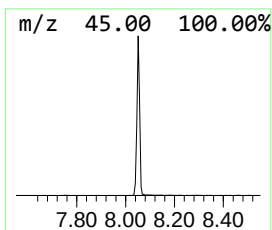
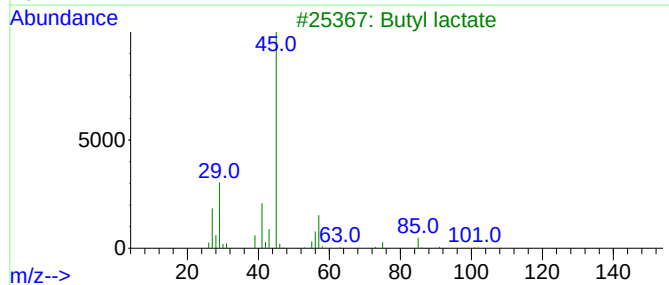
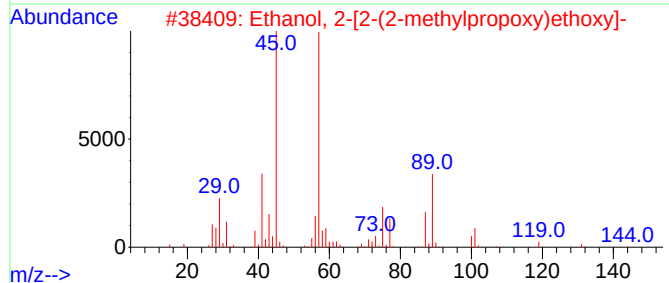
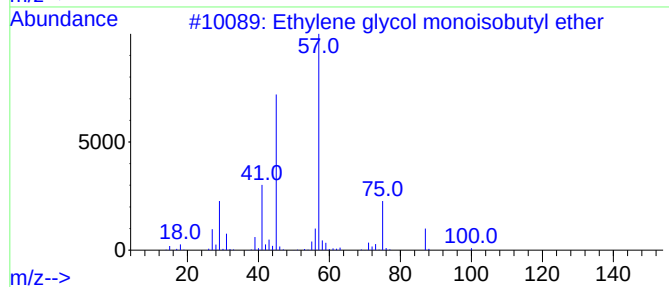
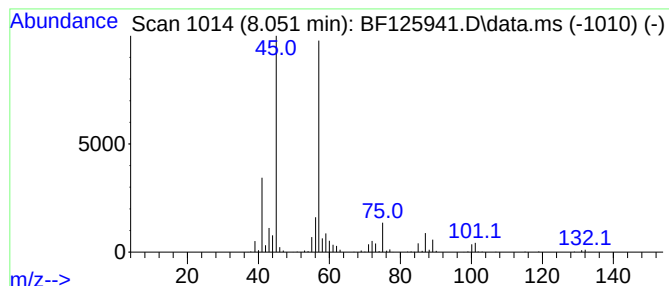
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethylene glycol monoisobuty... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	16.93 ng	1243670	Naphthalene-d8	8.145

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
2		Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3		Butyl lactate	146	C7H14O3	000138-22-7	50
4		Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5		Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	50



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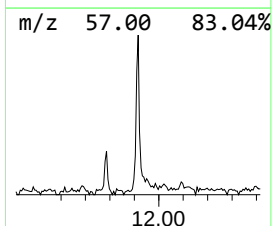
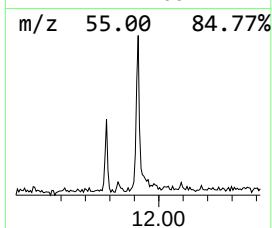
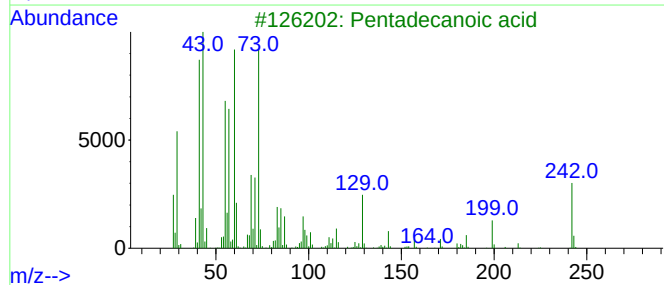
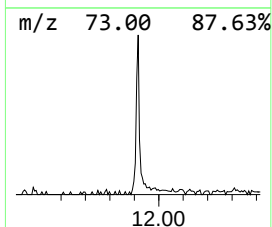
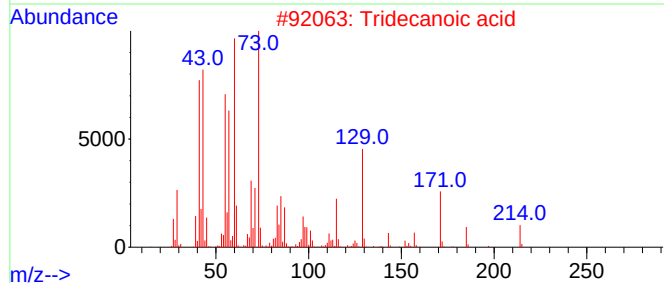
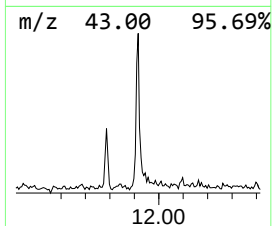
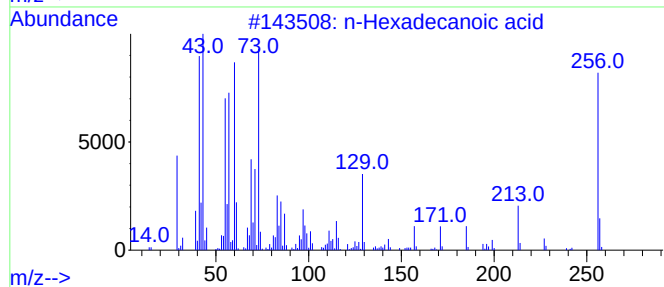
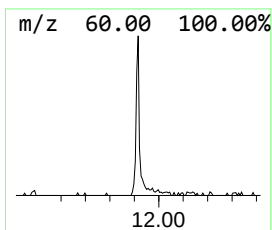
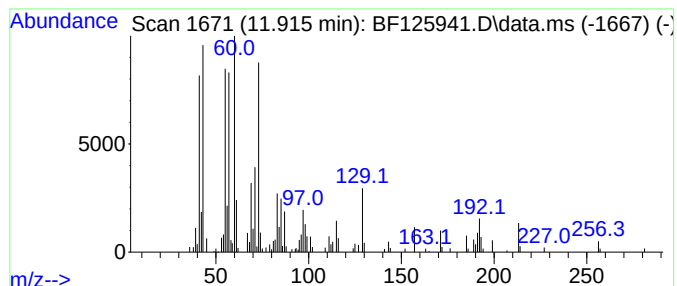
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.01 ng	243170	Phenanthrene-d10	11.386

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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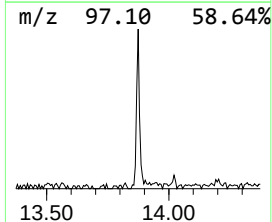
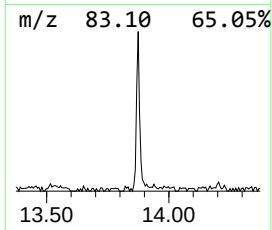
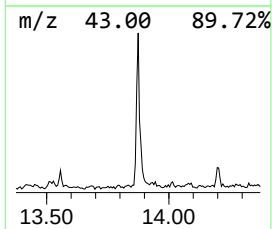
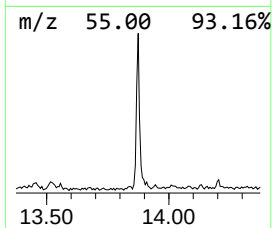
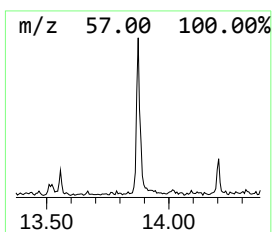
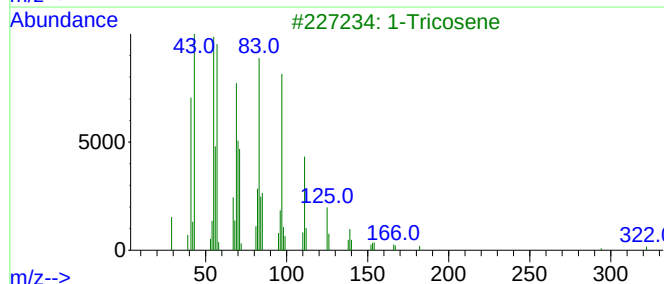
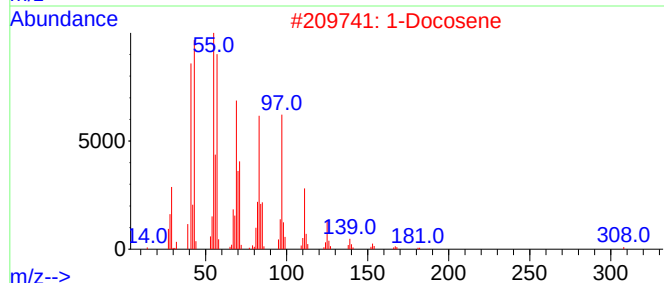
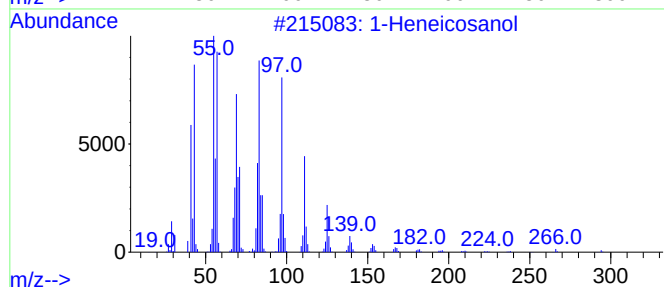
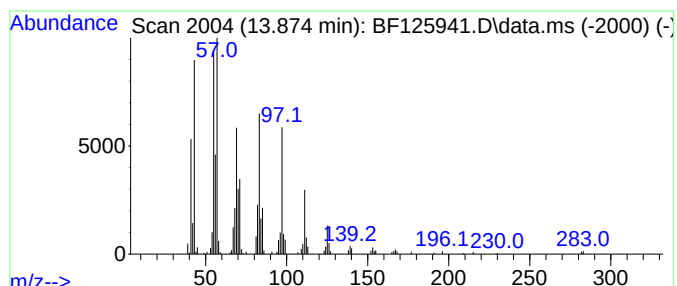
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.25 ng	312349	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			1-Docosene	308	C22H44	001599-67-3	90
3			1-Tricosene	322	C23H46	018835-32-0	87
4			1-Heptacosanol	396	C27H56O	002004-39-9	87
5			1-Hexacosene	364	C26H52	018835-33-1	87



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Sample : M4340-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

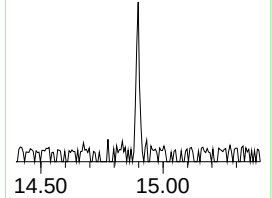
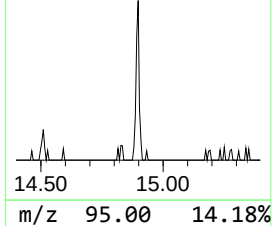
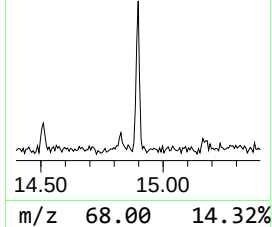
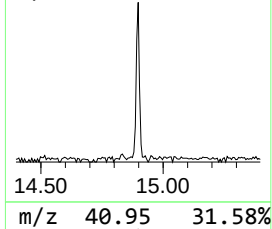
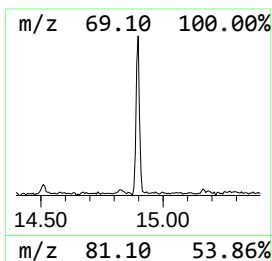
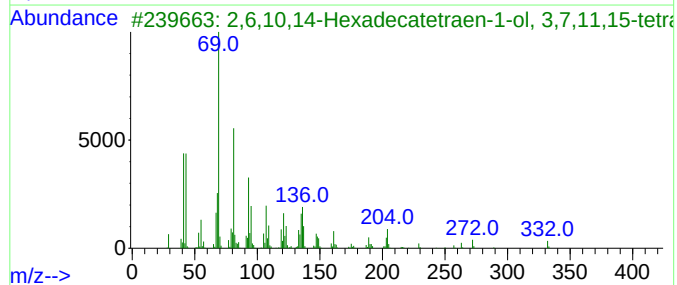
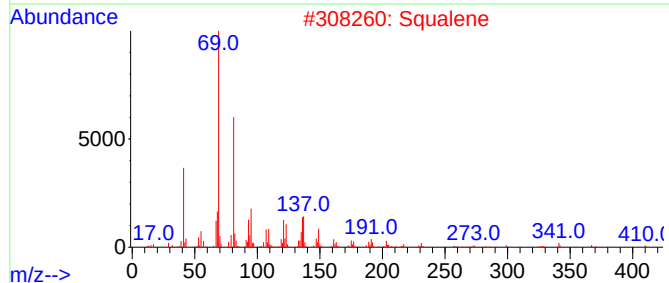
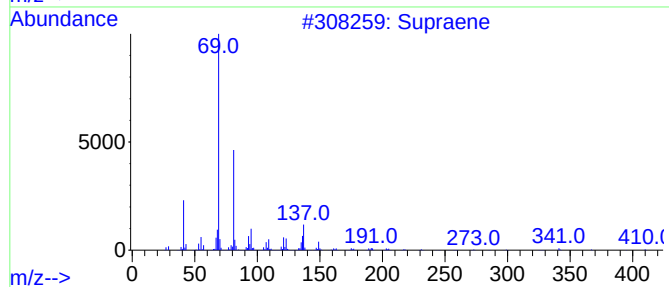
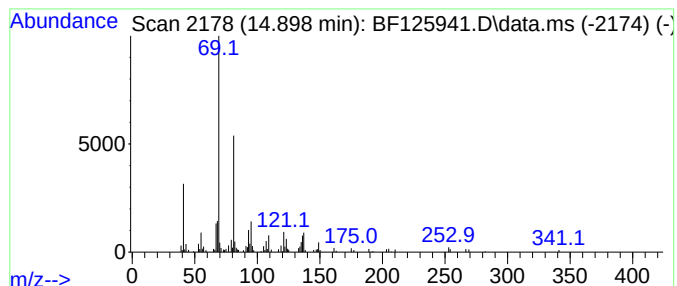
Instrument :
BNA_F
ClientSampleId :
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.898	2.96 ng	144040	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



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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...	2.157	59.8	ng	3344310	1	6.869	1118360	20.0
Ethylene glycol...	8.051	16.9	ng	1243670	2	8.145	1469510	20.0
n-Hexadecanoic ...	11.916	3.0	ng	243170	4	11.386	1613500	20.0
1-Heneicosanol	13.874	6.3	ng	312349	5	14.021	999939	20.0
Supraene	14.898	3.0	ng	144040	6	15.492	972219	20.0