

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
 Data File : BF125188.D
 Acq On : 24 Aug 2021 16:44
 Operator : JU/CG
 Sample : M3521-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124027

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: BF125188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	29	rVB	1282135	1645682	35.64%	4.546%
2	5.157	518	522	528	rVB	44326	54318	1.18%	0.150%
3	5.534	581	586	589	rBV	4178652	4562719	98.81%	12.603%
4	6.540	751	757	760	rBV	4074740	4617504	100.00%	12.755%
5	6.916	817	821	824	rBV	1090394	933703	20.22%	2.579%
6	7.475	911	916	919	rBV	2936720	3044437	65.93%	8.410%
7	8.092	1018	1021	1035	rBV	420806	500507	10.84%	1.383%
8	8.198	1035	1039	1042	rBV	1399359	1236971	26.79%	3.417%
9	9.269	1216	1221	1224	rBV	4816153	4296080	93.04%	11.867%
10	9.951	1333	1337	1340	rBV	1734014	1409578	30.53%	3.894%
11	10.251	1385	1388	1393	rVB	74935	74309	1.61%	0.205%
12	10.739	1466	1471	1474	rBV	3898994	3678521	79.66%	10.161%
13	11.239	1552	1556	1562	rBV	135310	140489	3.04%	0.388%
14	11.439	1586	1590	1592	rBV	1654433	1458193	31.58%	4.028%
15	11.457	1592	1593	1597	rVB	134486	103582	2.24%	0.286%
16	11.822	1652	1655	1658	rBV	69410	56585	1.23%	0.156%
17	11.957	1673	1678	1686	rBV	599329	591355	12.81%	1.633%
18	12.533	1770	1776	1780	rVB2	135312	134391	2.91%	0.371%
19	12.651	1792	1796	1800	rBV	244800	221910	4.81%	0.613%
20	12.739	1808	1811	1816	rBV	198392	194056	4.20%	0.536%
21	12.880	1829	1835	1840	rBV	192467	201394	4.36%	0.556%
22	13.022	1855	1859	1863	rBV	3942140	3939141	85.31%	10.881%
23	13.945	2013	2016	2018	rBV	76788	97896	2.12%	0.270%
24	14.051	2031	2034	2036	rBV	244742	274602	5.95%	0.759%
25	14.074	2036	2038	2041	rVV	1132879	1065275	23.07%	2.943%
26	14.098	2041	2042	2047	rVB	89896	76773	1.66%	0.212%
27	14.933	2181	2184	2188	rBV	114016	123502	2.67%	0.341%
28	15.127	2214	2217	2226	rVB	71444	139879	3.03%	0.386%
29	15.445	2267	2271	2274	rBV	42349	50145	1.09%	0.139%
30	15.504	2278	2281	2286	rVB	58456	76968	1.67%	0.213%
31	15.574	2287	2293	2303	rBV2	843474	1151577	24.94%	3.181%
32	16.051	2370	2374	2378	rBV4	36699	50158	1.09%	0.139%

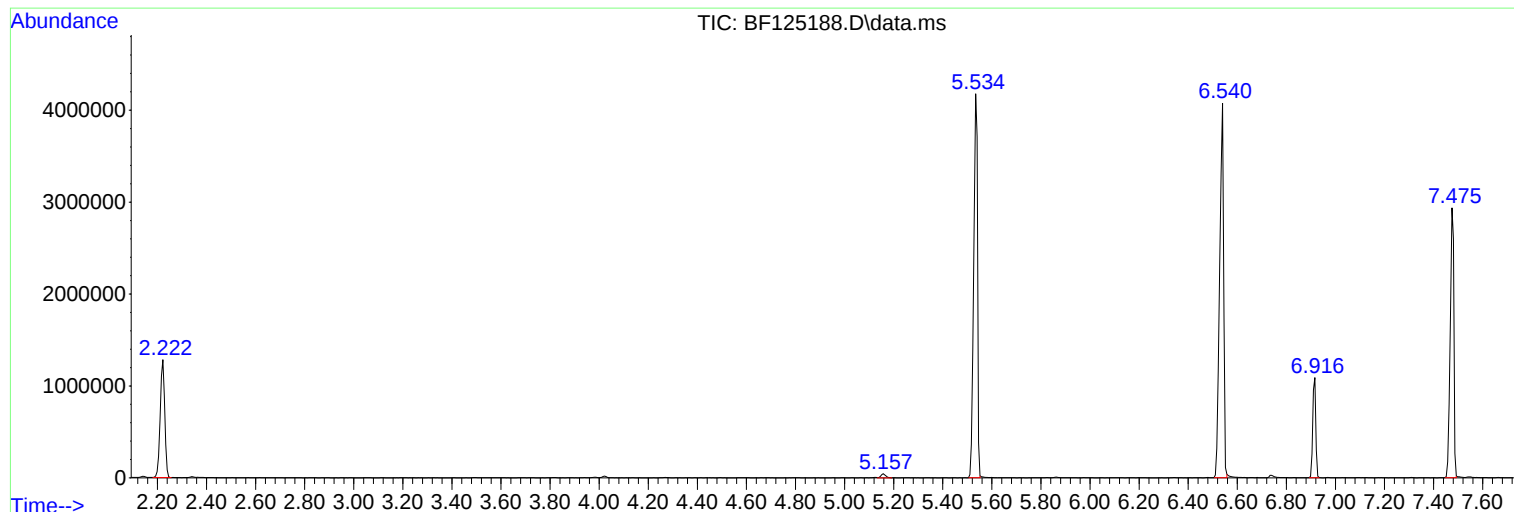
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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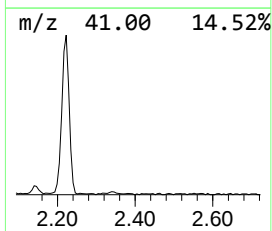
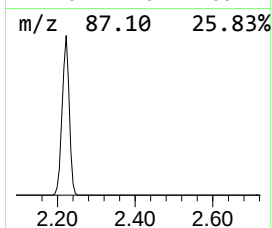
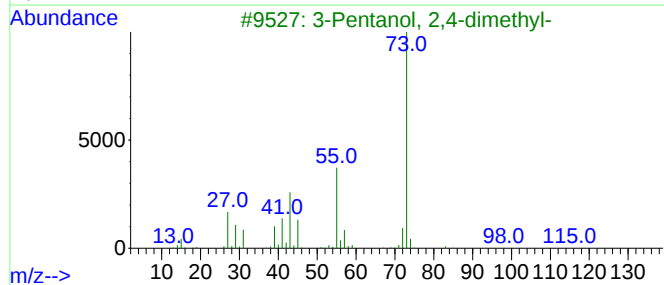
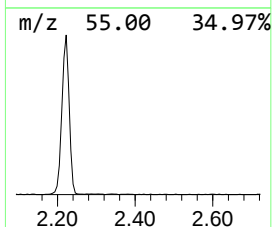
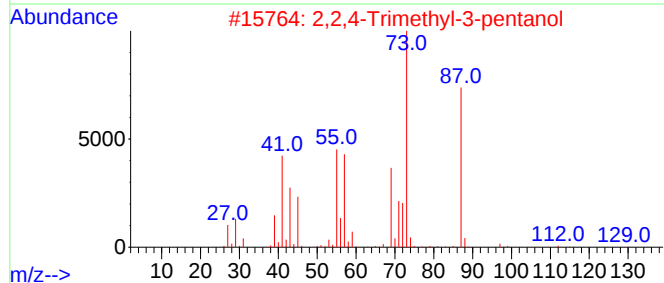
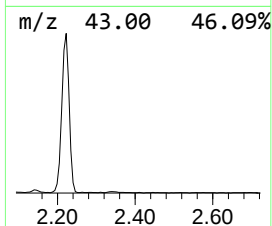
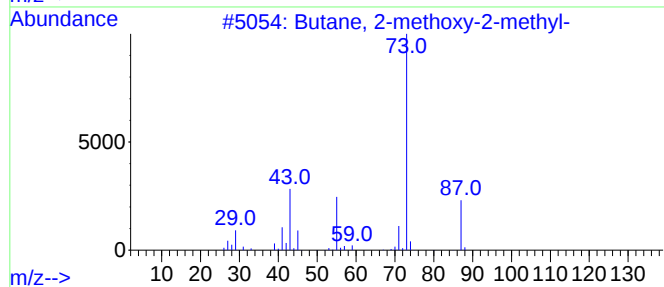
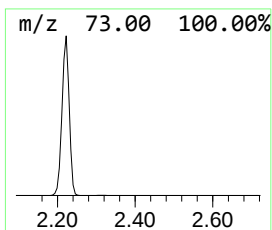
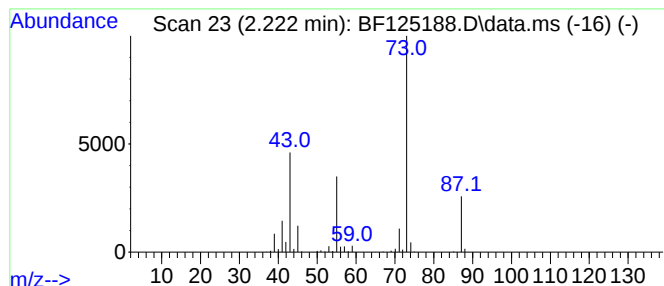
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	35.25 ng	1645680	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23



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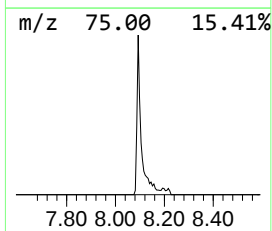
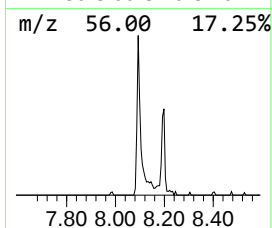
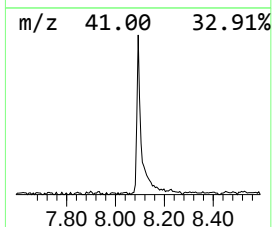
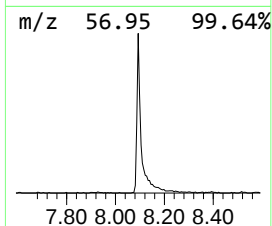
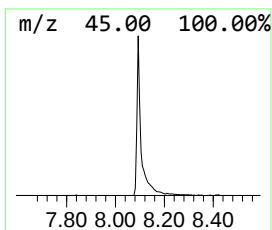
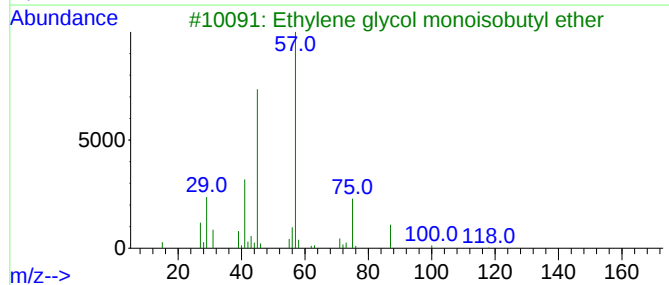
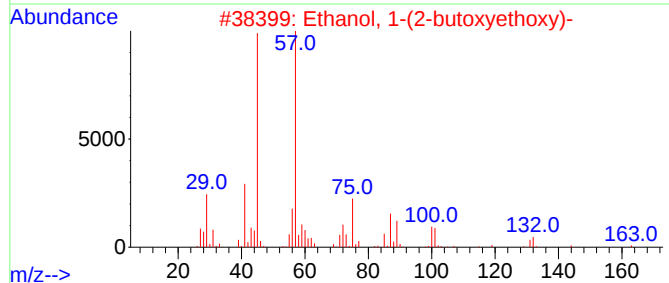
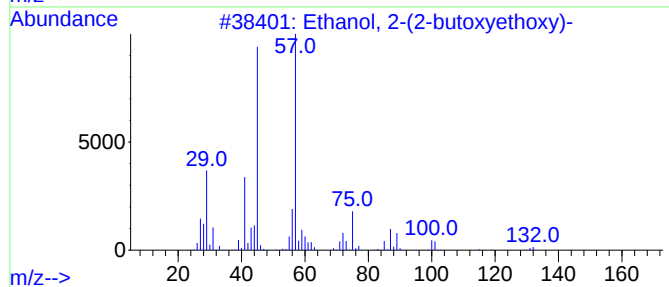
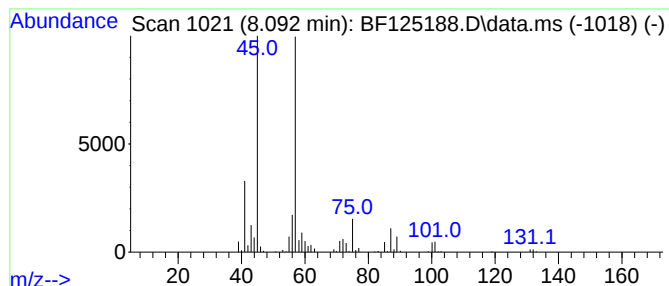
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	8.09 ng	500507	Naphthalene-d8	8.198

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	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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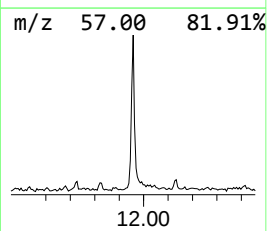
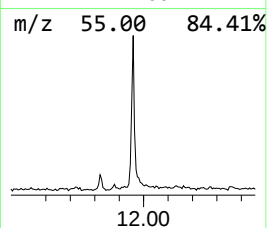
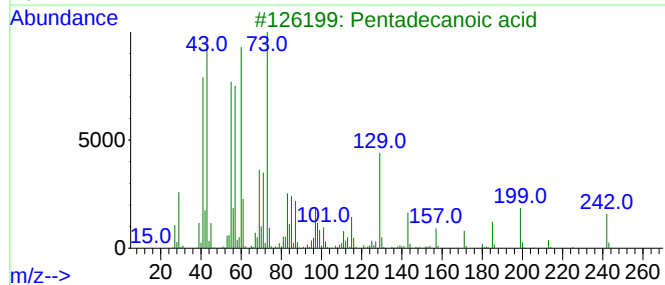
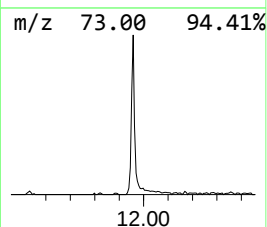
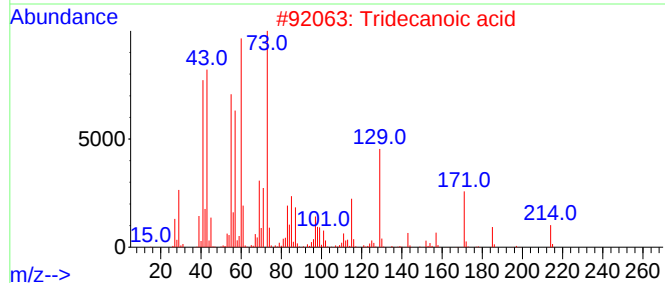
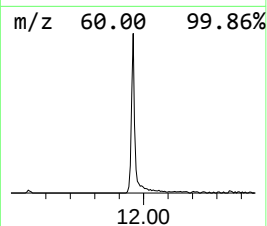
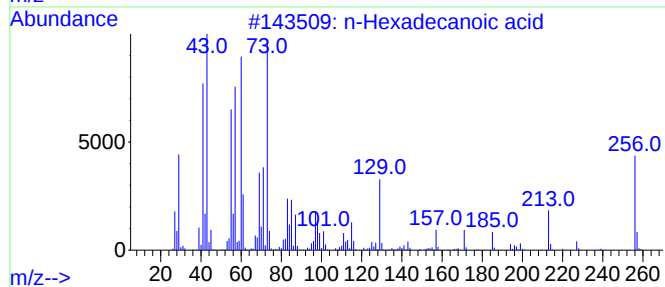
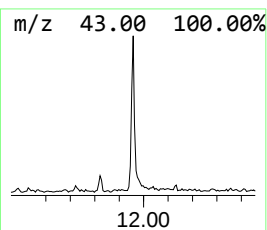
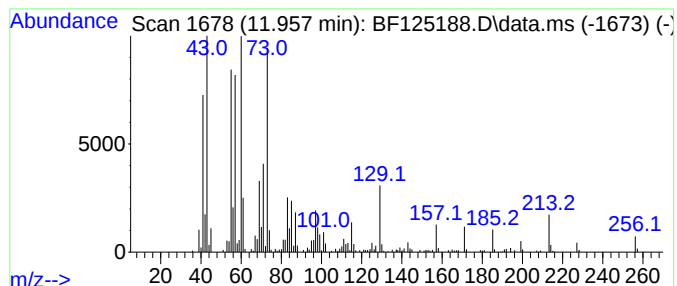
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	8.11 ng	591355	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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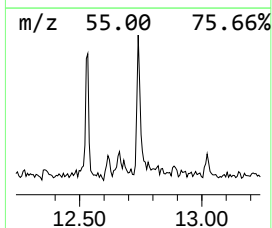
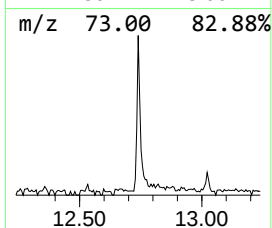
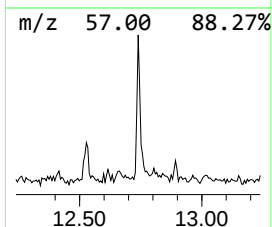
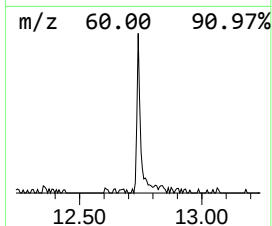
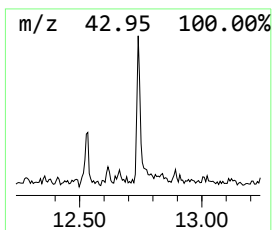
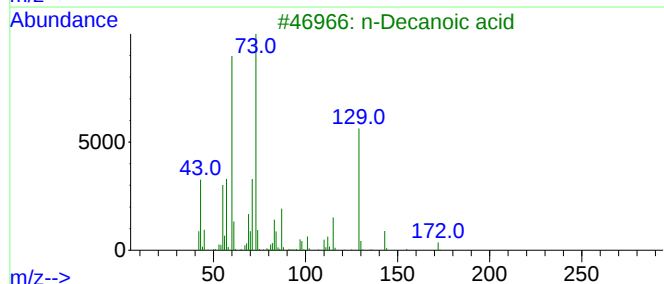
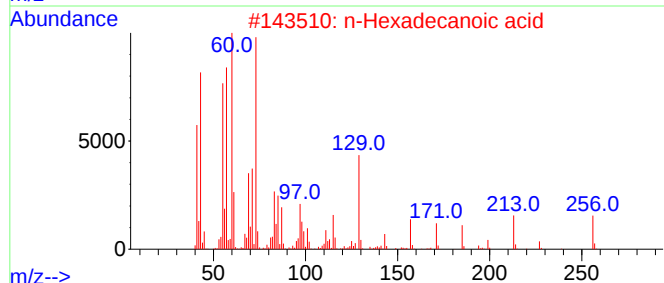
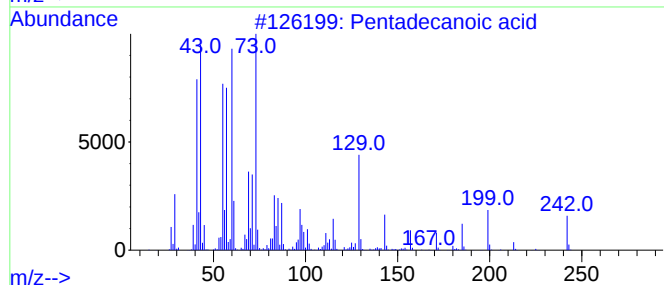
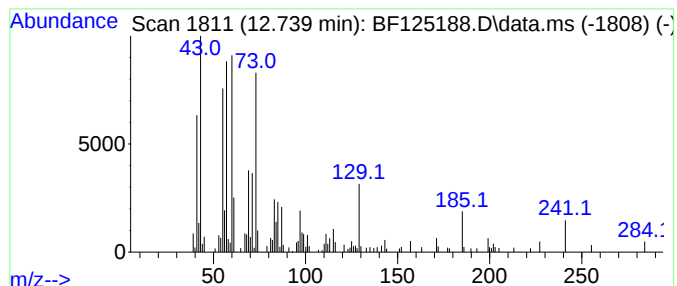
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Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.66 ng	194056	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			n-Decanoic acid	172	C10H20O2	000334-48-5	83
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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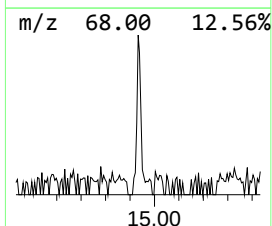
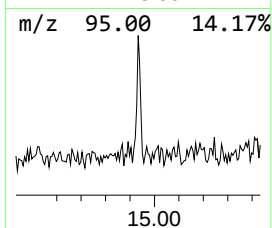
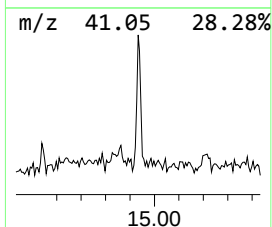
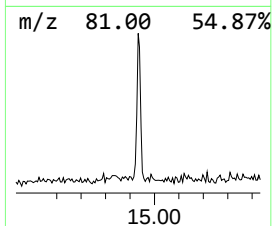
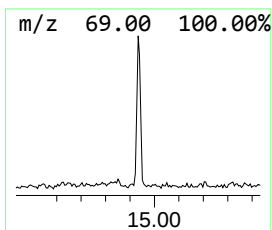
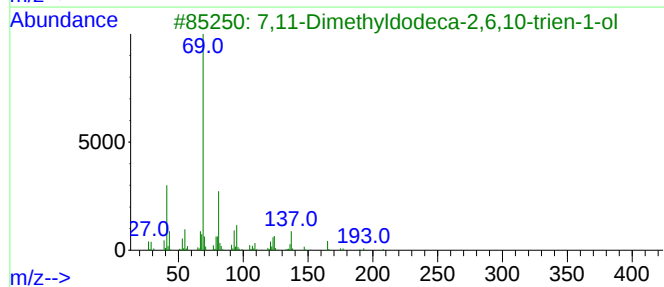
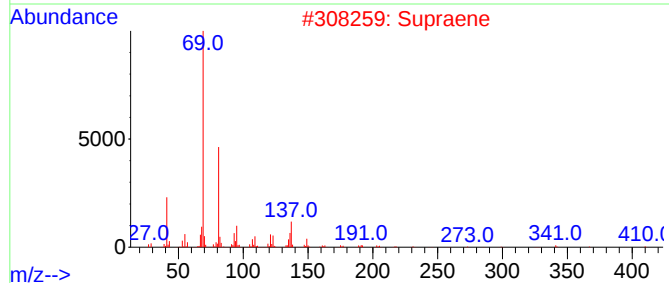
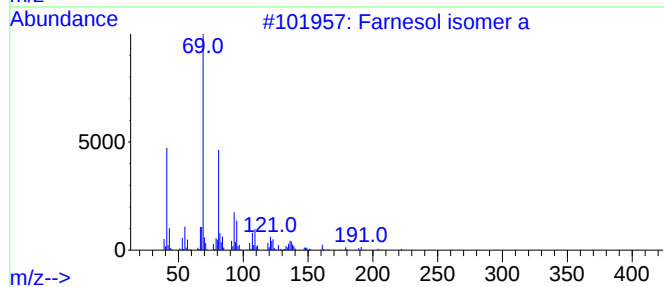
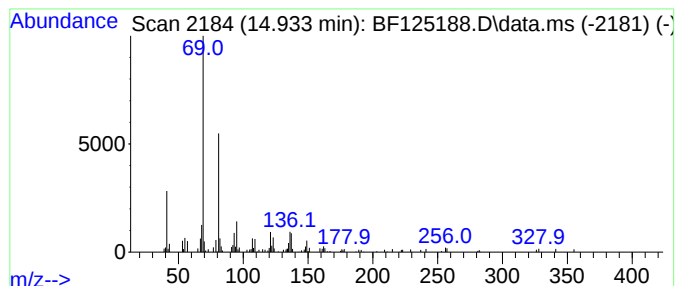
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Peak Number 5 Farnesol isomer a Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.14 ng	123502	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	87
2			Supraene	410	C30H50	007683-64-9	83
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



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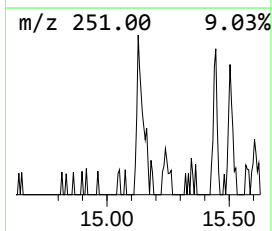
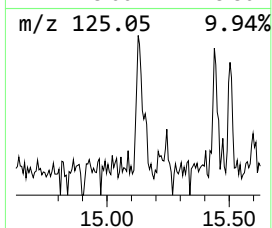
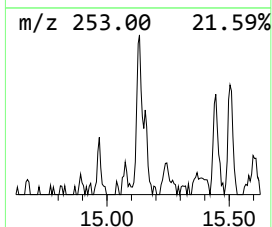
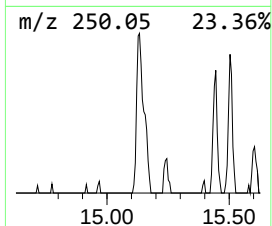
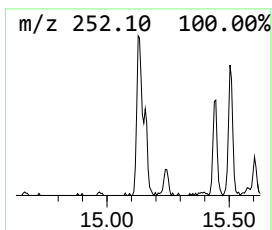
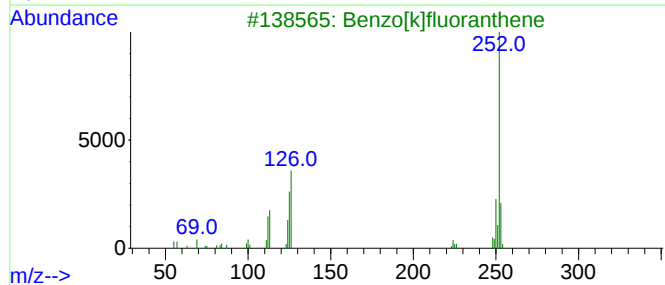
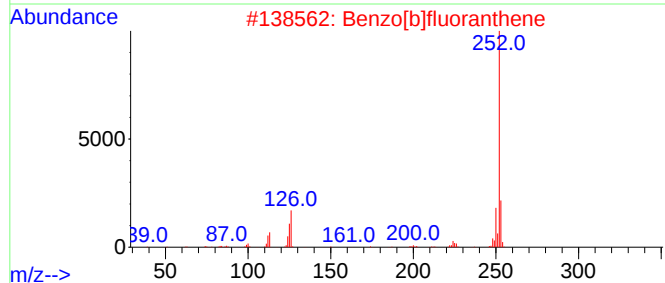
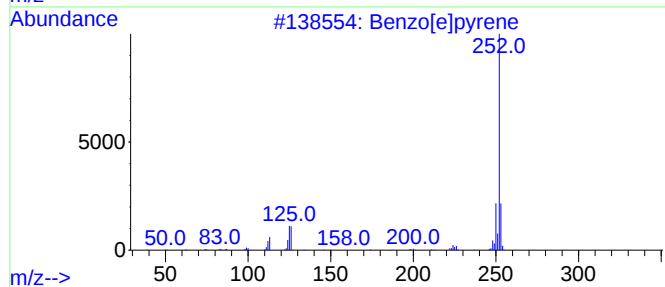
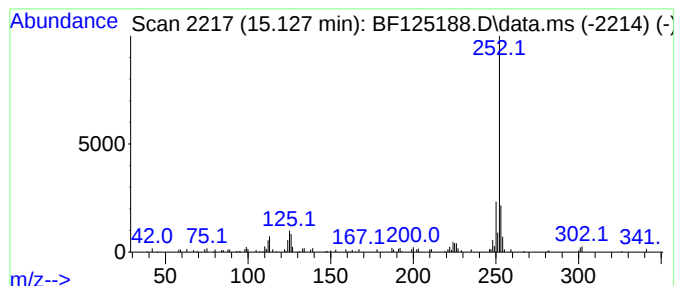
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.43 ng	139879	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Perylene	252	C20H12	000198-55-0	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125188.D
Acq On : 24 Aug 2021 16:44
Operator : JU/CG
Sample : M3521-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124027

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...	2.222	35.3	ng	1645680	1	6.916	933703	20.0
Ethanol, 2-(2-b...	8.092	8.1	ng	500507	2	8.198	1236970	20.0
n-Hexadecanoic ...	11.957	8.1	ng	591355	4	11.439	1458190	20.0
Pentadecanoic acid	12.739	2.7	ng	194056	4	11.439	1458190	20.0
Farnesol isomer a	14.933	2.1	ng	123502	6	15.574	1151580	20.0
Benzo[e]pyrene	15.127	2.4	ng	139879	6	15.574	1151580	20.0