LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126025.D
Acq On : 3 Nov 2021 18:16
Operator : JU/CG
Sample : M4470-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126025.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	4	11	16	rVB	1649386	2011979	50.10%	6.304%
2	5.463	569	574	578	rBV	3221128	3247039	80.86%	10.174%
3	6.475	741	746	749	rBV	3442149	3355093	83.55%	10.513%
4	6.681	778	781	786	rBV2	32105	44148	1.10%	0.138%
5	6.851	806	810	813	rBV	1185974	988242	24.61%	3.097%
6	7.410	900	905	908	rBV	2501056	2224215	55.39%	6.969%
7	8.039	1007	1012	1019	rBV	1207298	1217619	30.32%	3.815%
8	8.134	1023	1028	1030	rVV	1383045	1288120	32.08%	4.036%
9	8.151	1030	1031	1037	rVB	64763	49826	1.24%	0.156%
10	9.210	1205	1211	1214	rBV	4250087	4015821	100.00%	12.583%
11	9.886	1319	1326	1329	rBV	1769479	1502786	37.42%	4.709%
12	9.916	1329	1331	1335	rVB	55048	46662	1.16%	0.146%
13	10.086	1357	1360	1363	rVB	57151	48267	1.20%	0.151%
14	10.292	1392	1395	1398	rBV	90044	110178	2.74%	0.345%
15	10.669	1455	1459	1462	rBV	3199674	2627443	65.43%	8.233%
16	10.792	1477	1480	1481	rBV	61605	50195	1.25%	0.157%
17	11.116	1531	1535	1541	rVB	445483	484018	12.05%	1.517%
18	11.269	1558	1561	1564	rVB2	50815	57829	1.44%	0.181%
19	11.369	1574	1578	1580	rBV	1686157	1434011	35.71%	4.493%
20	11.392	1580	1582	1585	rVV	390260	313643	7.81%	0.983%
21	11.439	1588	1590	1593	rVB	99019	82256	2.05%	0.258%
22	11.474	1593	1596	1599	rBV5	39487	59828	1.49%	0.187%
23	11.669	1626	1629	1632	rBV3	67665	76022	1.89%	0.238%
24	11.763	1643	1645	1651	rVB2	106825	95534	2.38%	0.299%
25	11.898	1665	1668	1671	rBV	262662	211436	5.27%	0.663%
26	12.074	1696	1698	1703	rVB2	154647	174649	4.35%	0.547%
27	12.574	1781	1783	1787	rVB	381770	343193	8.55%	1.075%
28	12.804	1820	1822	1825	rVB	311531	253057	6.30%	0.793%
29	12.957	1844	1848	1851	rBV	3420438	3042120	75.75%	9.532%
30	13.498	1938	1940	1944	rVB	232636	218477	5.44%	0.685%
31	14.004	2022	2026	2029	rBV	1030011	1043714	25.99%	3.270%
32	14.868	2170	2173	2183	rVB	218791	321548	8.01%	1.008%
33	15.468	2271	2275	2279	rBV2	695851	788837	19.64%	2.472%
34	18.374	2763	2769	2771	rBV6	41635	86260	2.15%	0.270%

Sum of corrected areas: 31914065

Instrument :
BNA_F
ClientSampleId :
TP-1

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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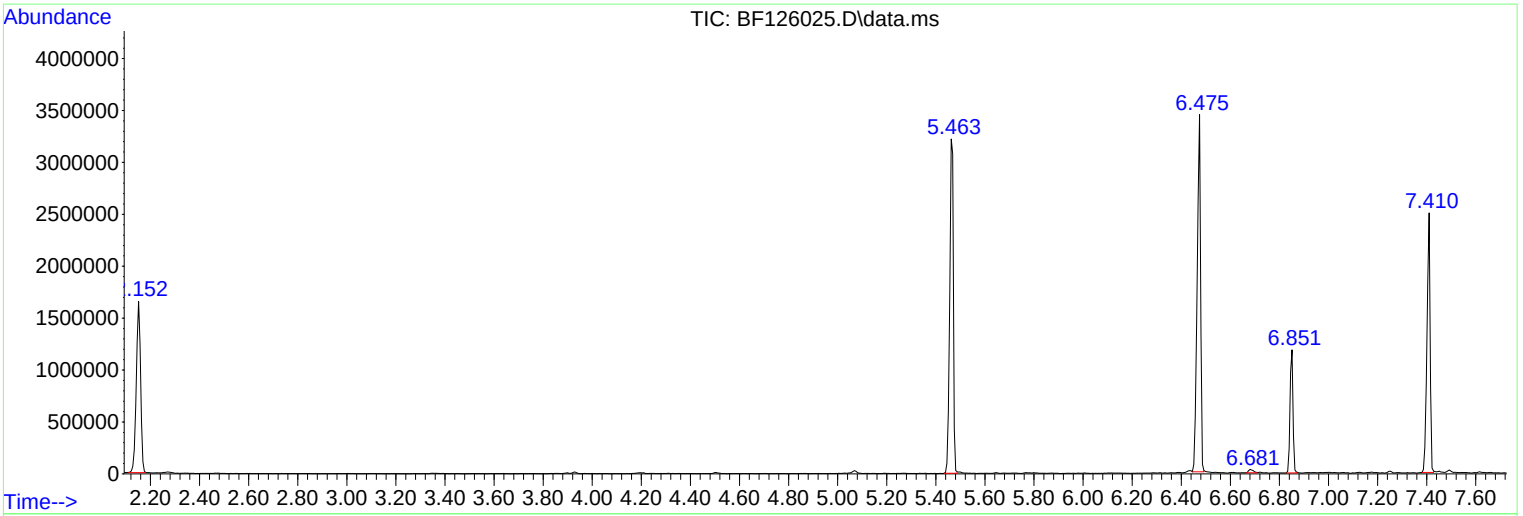
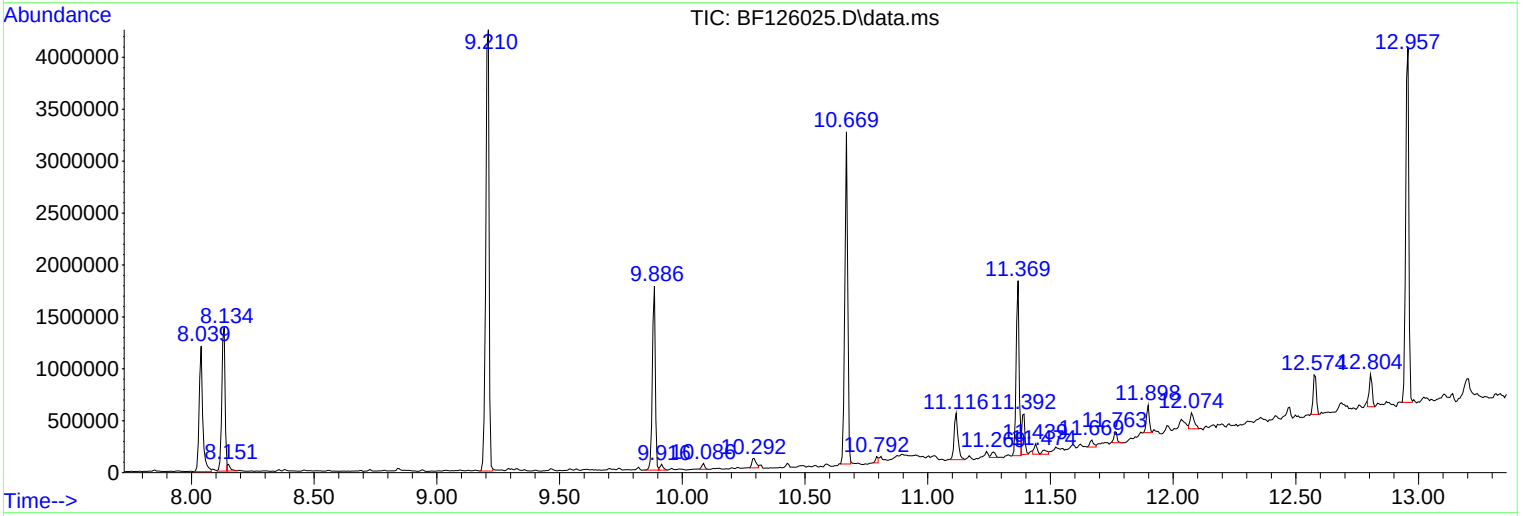
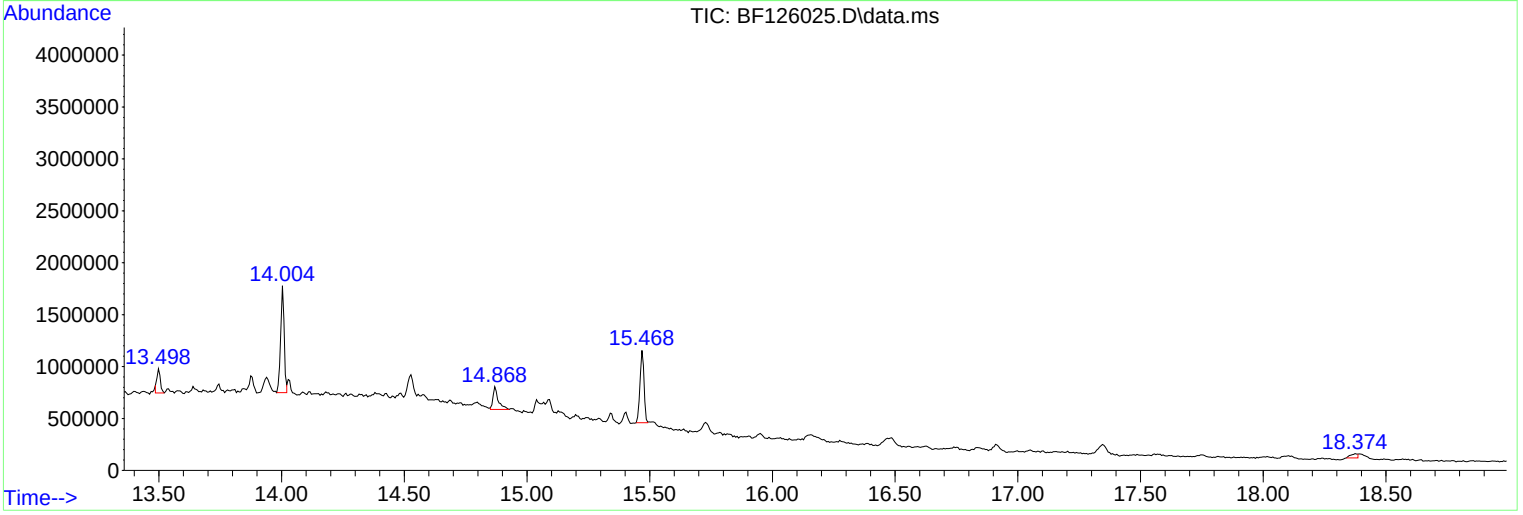
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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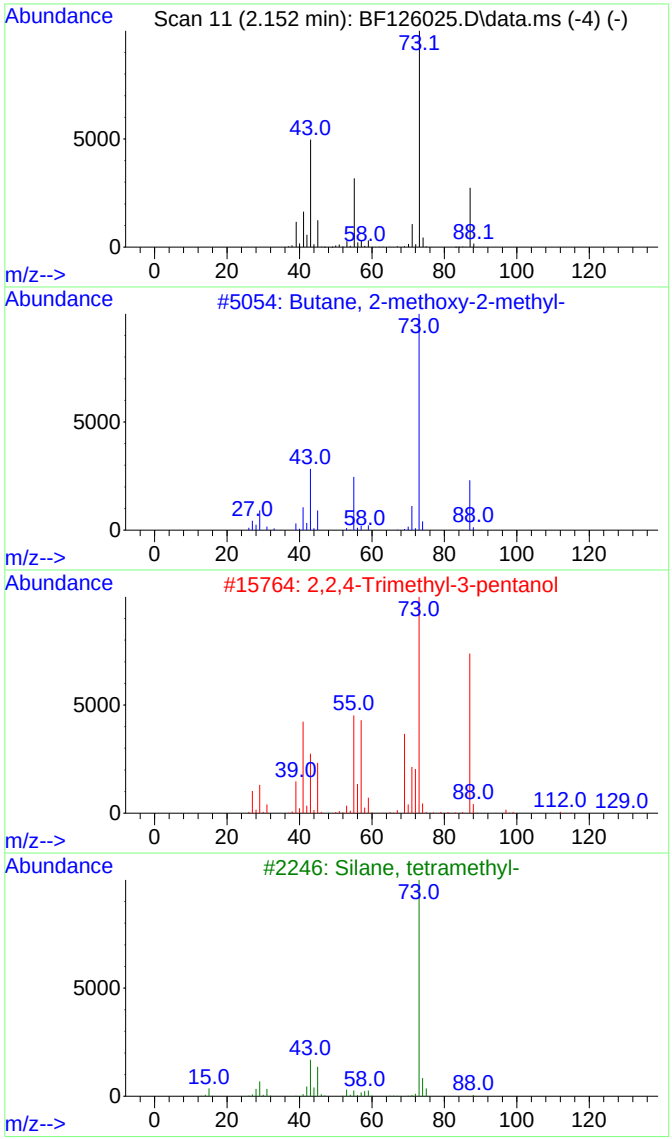
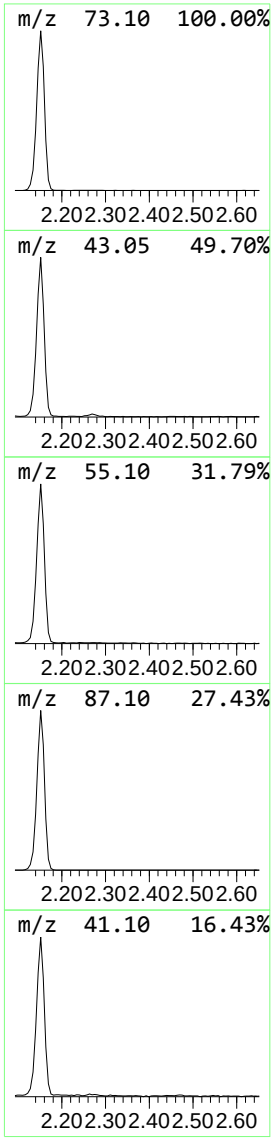
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	40.72 ng	2011980	1,4-Dichlorobenzene-d4	6.851

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	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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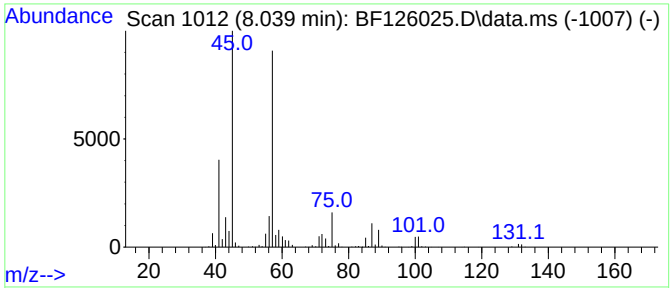
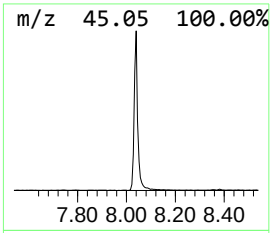
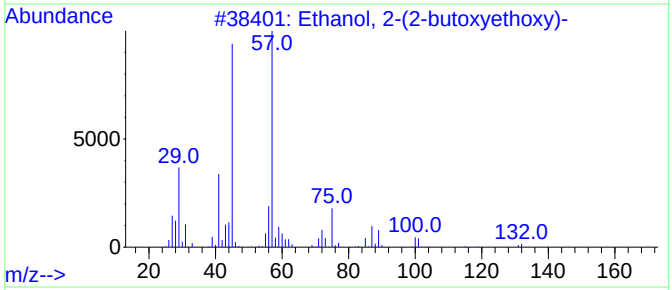
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

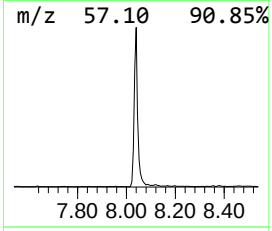
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	18.91 ng	1217620	Naphthalene-d8	8.134

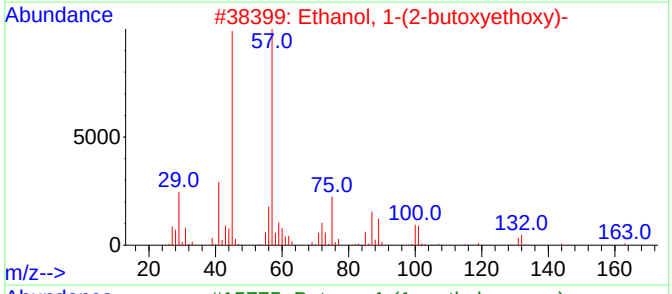
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50

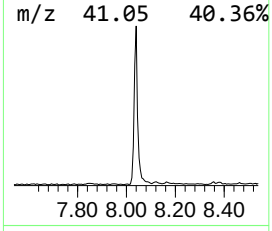


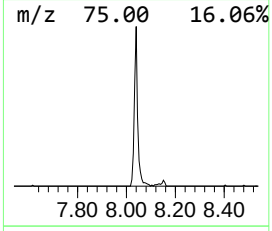


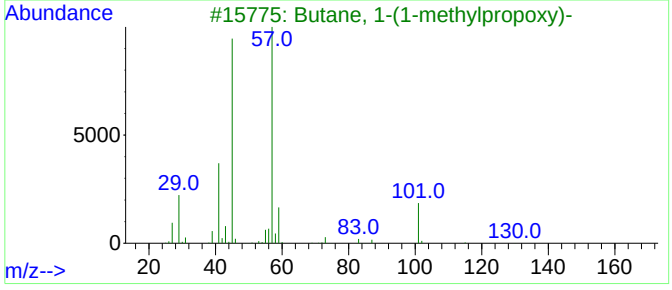


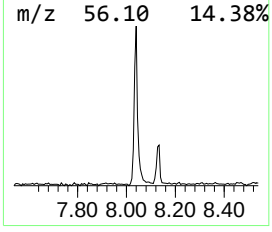












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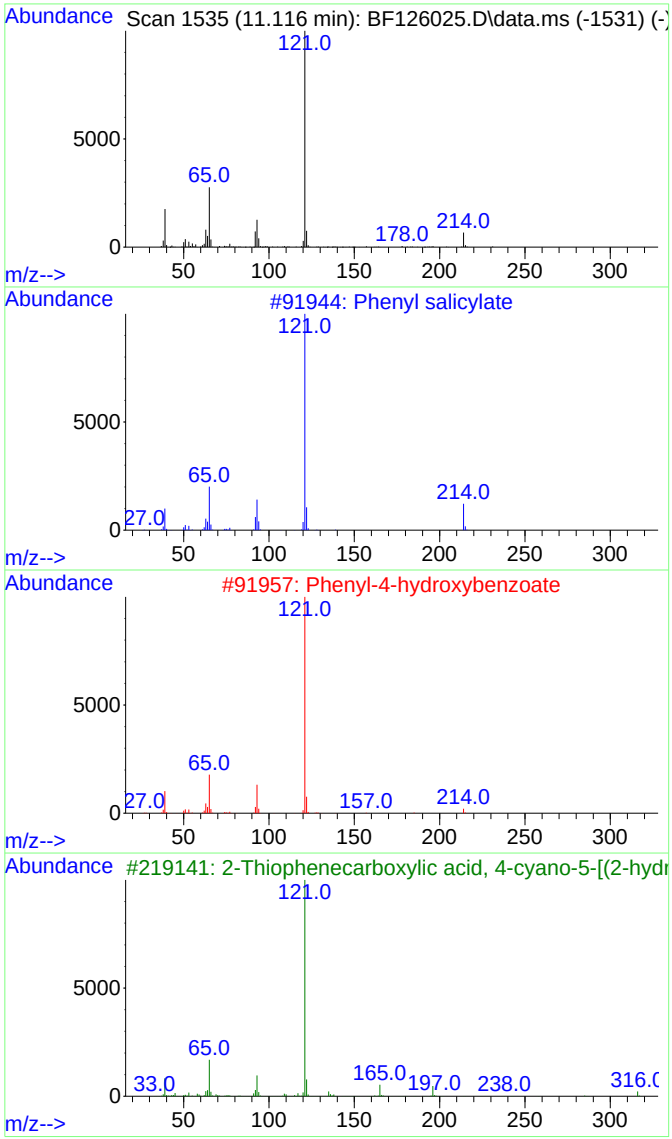
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

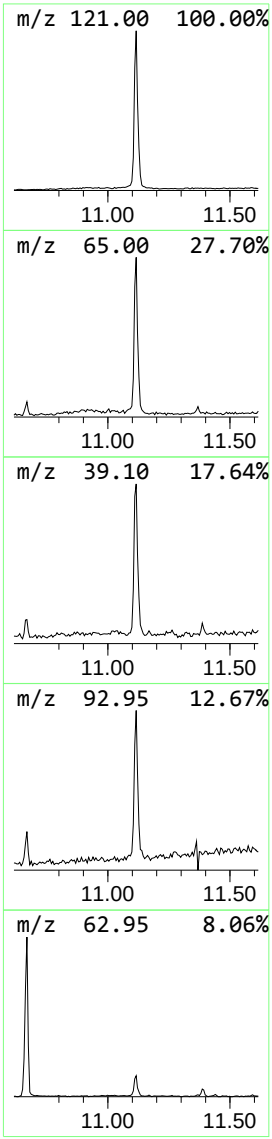
****

Peak Number 3 Phenyl salicylate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.116	6.75 ng	484018	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl salicylate	214	C13H10O3	000118-55-8	97
2	Phenyl-4-hydroxybenzoate	214	C13H10O3	017696-62-7	91
3	2-Thiophenecarboxylic acid, 4-cy...	316	C15H12N2O4S	1000337-61-4	83
4	(p-Hydroxyphenyl)glyoxal	150	C8H6O3	024645-80-5	78
5	Methylparaben	152	C8H8O3	000099-76-3	72





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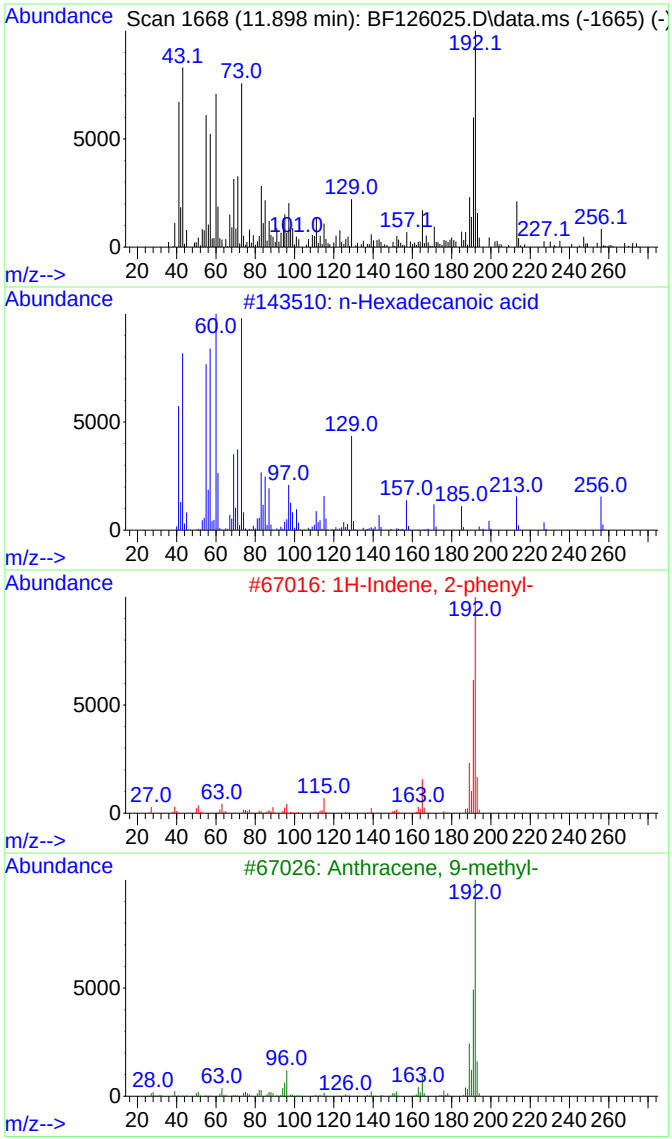
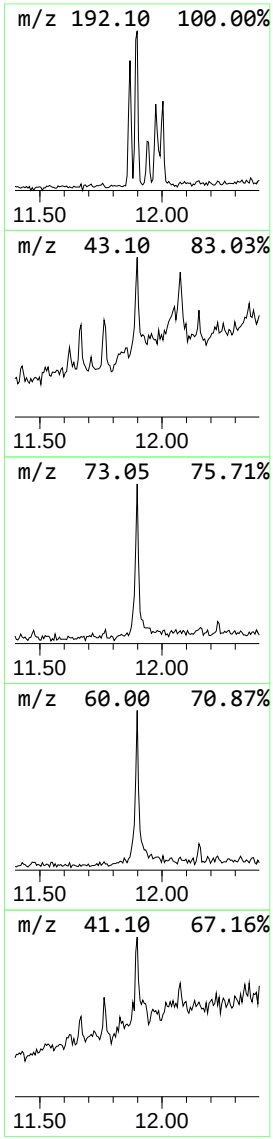
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	2.95 ng	211436	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	42
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	42
5	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	42





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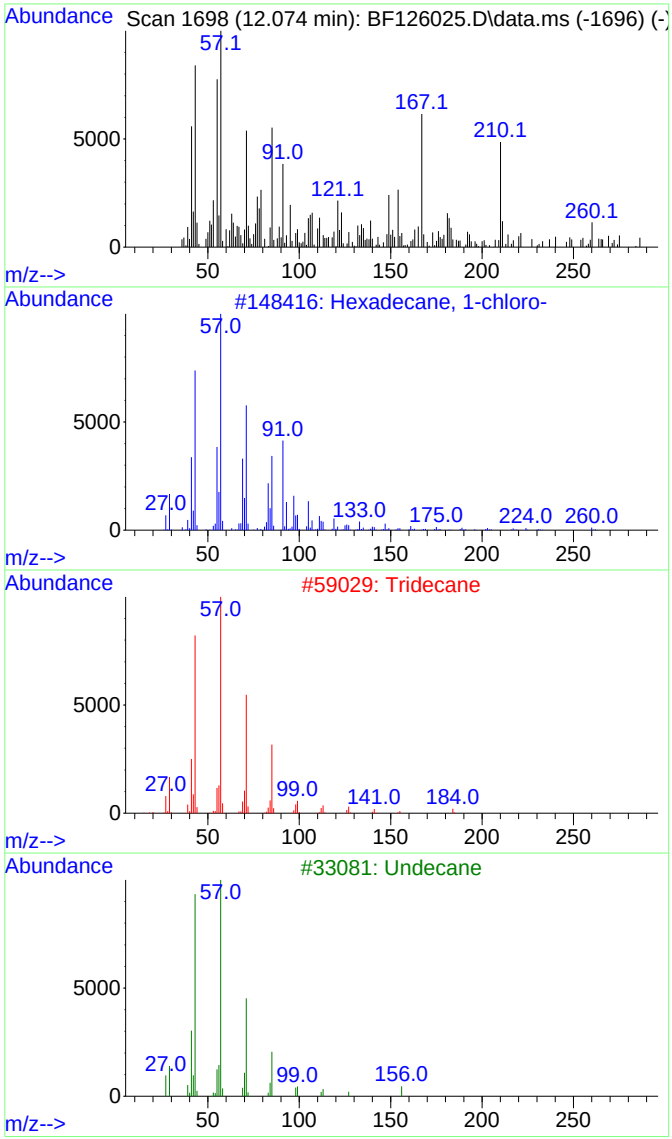
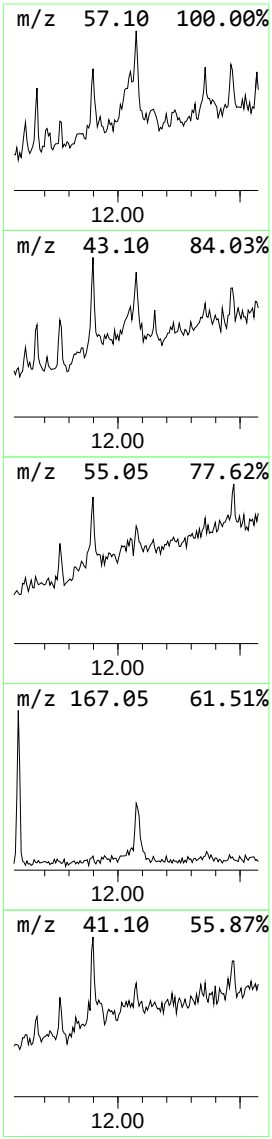
****

Peak Number 5 unknown12.074 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.074	2.44 ng	174649	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	35
2	Tridecane	184	C13H28	000629-50-5	25
3	Undecane	156	C11H24	001120-21-4	25
4	Heptadecane	240	C17H36	000629-78-7	25
5	Octadecane	254	C18H38	000593-45-3	20





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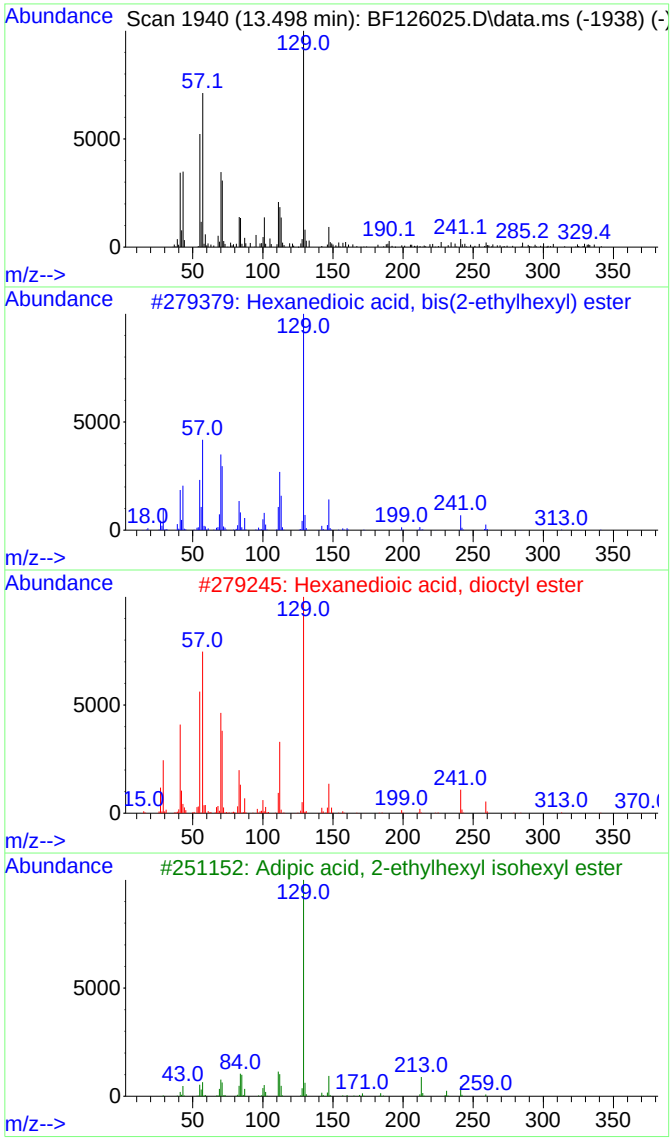
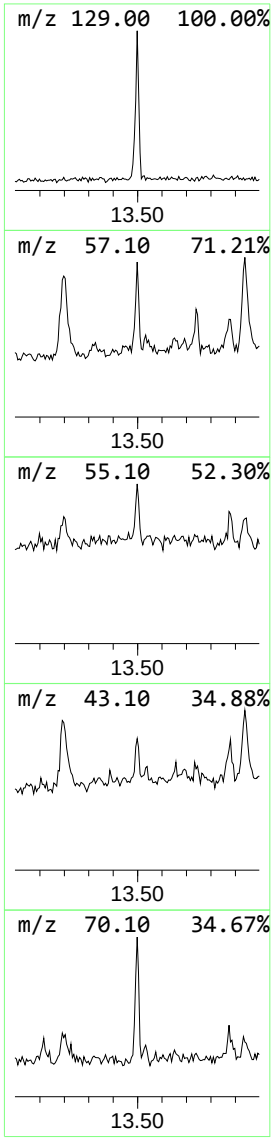
****
Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	4.19 ng	218477	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	50
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	49
3	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	47
4	Adipic acid, isohexyl 2-methylbu...	300	C17H32O4	1000324-67-4	47
5	Adipic acid, cycloheptyl octyl e...	354	C21H38O4	1000324-72-1	47





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TIC Library : C:\Database\NIST20.L
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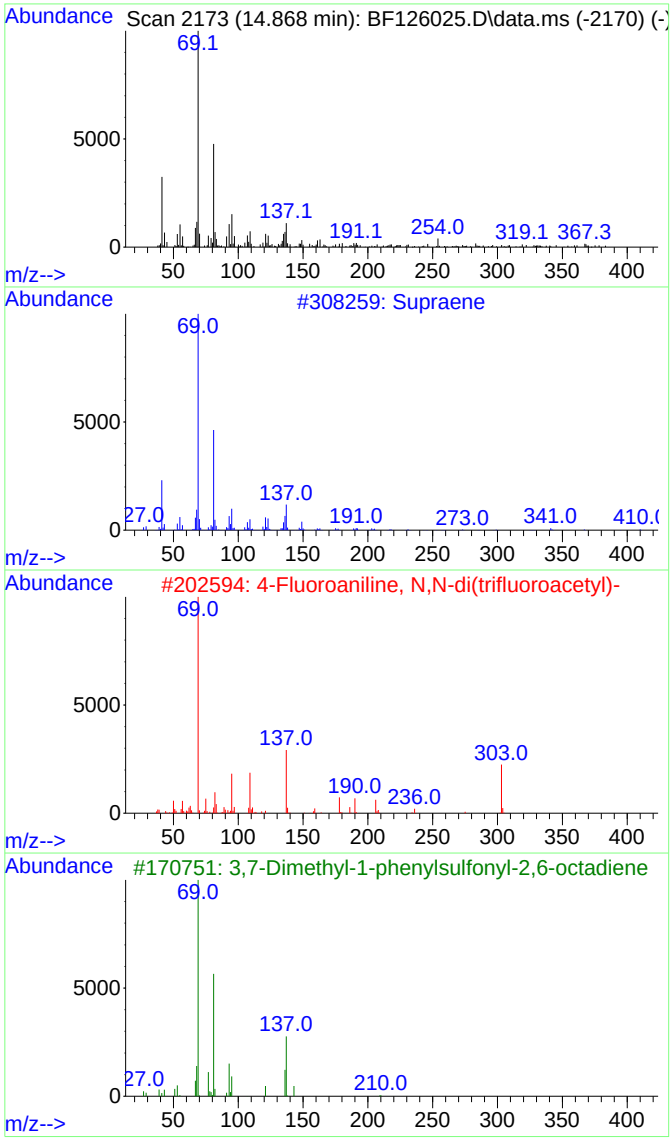
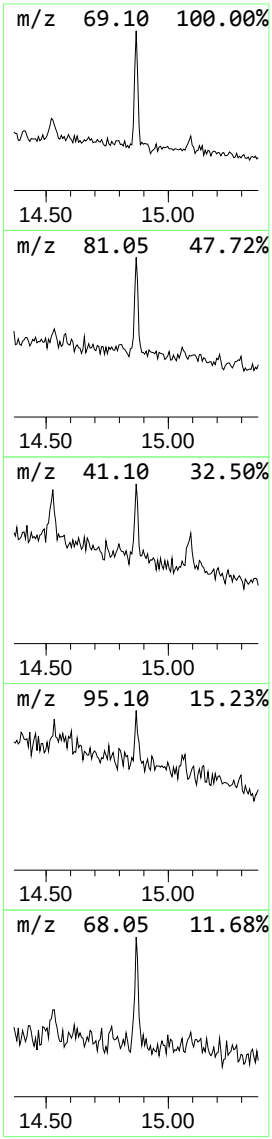
Peak Number 7 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	8.15 ng	321548	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	4-Fluoroaniline, N,N-di(trifluor...	303	C10H4F7NO2	1000328-30-6	64
3	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

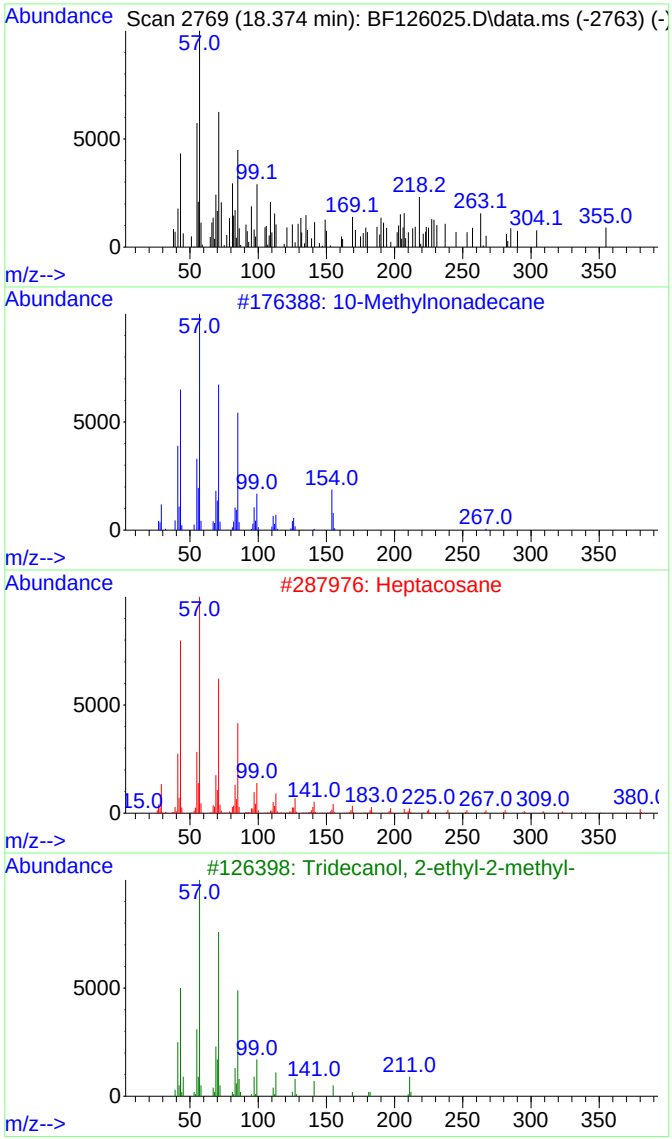
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

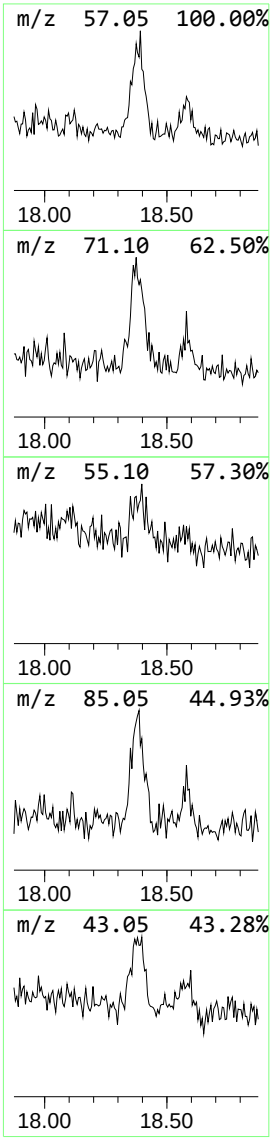
****

Peak Number 8 unknown18.374 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	2.19 ng	86260	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	35
2	Heptacosane	380	C27H56	000593-49-7	35
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	35
4	Docosane	310	C22H46	000629-97-0	35
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126025.D
Acq On : 3 Nov 2021 18:16
Operator : JU/CG
Sample : M4470-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.152	40.7	ng	2011980	1	6.851	988242	20.0
Ethanol, 2-(2-b...	8.039	18.9	ng	1217620	2	8.134	1288120	20.0
Phenyl salicylate	11.116	6.8	ng	484018	4	11.369	1434010	20.0
n-Hexadecanoic ...	11.898	3.0	ng	211436	4	11.369	1434010	20.0
unknown12.074	12.074	2.4	ng	174649	4	11.369	1434010	20.0
Hexanedioic aci...	13.498	4.2	ng	218477	5	14.004	1043710	20.0
Supraene	14.868	8.2	ng	321548	6	15.468	788837	20.0
unknown18.374	18.374	2.2	ng	86260	6	15.468	788837	20.0