LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126042.D
Acq On : 4 Nov 2021 13:17
Operator : JU/CG
Sample : M4448-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-224

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: BF126042.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	4	12	17	rBV	1551789	1975543	37.16%	5.235%
2	5.469	570	575	578	rBV	4302809	4103742	77.19%	10.874%
3	6.481	741	747	750	rBV	4167656	4352938	81.88%	11.535%
4	6.851	806	810	813	rBV	1170374	893008	16.80%	2.366%
5	7.410	900	905	908	rBV	2676805	2828458	53.21%	7.495%
6	8.039	1007	1012	1024	rBV	1120022	1123580	21.14%	2.977%
7	8.133	1024	1028	1031	rVV	1434901	1126133	21.18%	2.984%
8	9.210	1205	1211	1214	rBV	6651297	5316101	100.00%	14.087%
9	9.327	1227	1231	1235	rBV	204678	183210	3.45%	0.485%
10	9.886	1322	1326	1329	rBV	1619459	1342020	25.24%	3.556%
11	10.669	1455	1459	1463	rBV	3765590	3507665	65.98%	9.295%
12	11.369	1574	1578	1580	rBV	1584788	1319211	24.82%	3.496%
13	11.392	1580	1582	1584	rVV	147035	115129	2.17%	0.305%
14	11.439	1586	1590	1593	rVB3	68994	71445	1.34%	0.189%
15	11.763	1643	1645	1649	rBV	92001	76895	1.45%	0.204%
16	11.898	1665	1668	1672	rBV	229546	199160	3.75%	0.528%
17	12.468	1763	1765	1768	rVB	174667	153610	2.89%	0.407%
18	12.580	1777	1784	1787	rBV	366922	383079	7.21%	1.015%
19	12.804	1816	1822	1825	rBV	298069	317873	5.98%	0.842%
20	12.957	1844	1848	1851	rVB	5203281	4445654	83.63%	11.780%
21	13.021	1851	1859	1865	rVB8	28115	68896	1.30%	0.183%
22	13.192	1882	1888	1892	rBV8	61885	128634	2.42%	0.341%
23	13.868	2000	2003	2011	rVB2	153174	230943	4.34%	0.612%
24	14.004	2021	2026	2029	rBV	1007078	1119203	21.05%	2.966%
25	14.027	2029	2030	2033	rVB	148604	85497	1.61%	0.227%
26	14.639	2131	2134	2139	rBV7	66798	76380	1.44%	0.202%
27	14.868	2169	2173	2176	rBV	541748	540662	10.17%	1.433%
28	15.039	2198	2202	2205	rBV	132919	196516	3.70%	0.521%
29	15.339	2250	2253	2259	rVB	104647	114514	2.15%	0.303%
30	15.404	2260	2264	2268	rVB	114860	138422	2.60%	0.367%
31	15.468	2269	2275	2279	rBV	684725	878347	16.52%	2.327%
32	16.380	2426	2430	2436	rVB9	34074	67507	1.27%	0.179%
33	16.909	2516	2520	2528	rVB3	69872	138423	2.60%	0.367%
34	17.350	2590	2595	2602	rVB2	54294	119544	2.25%	0.317%

Sum of corrected areas: 37737942

Instrument :
BNA_F
ClientSampleId :
VNJ-224

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
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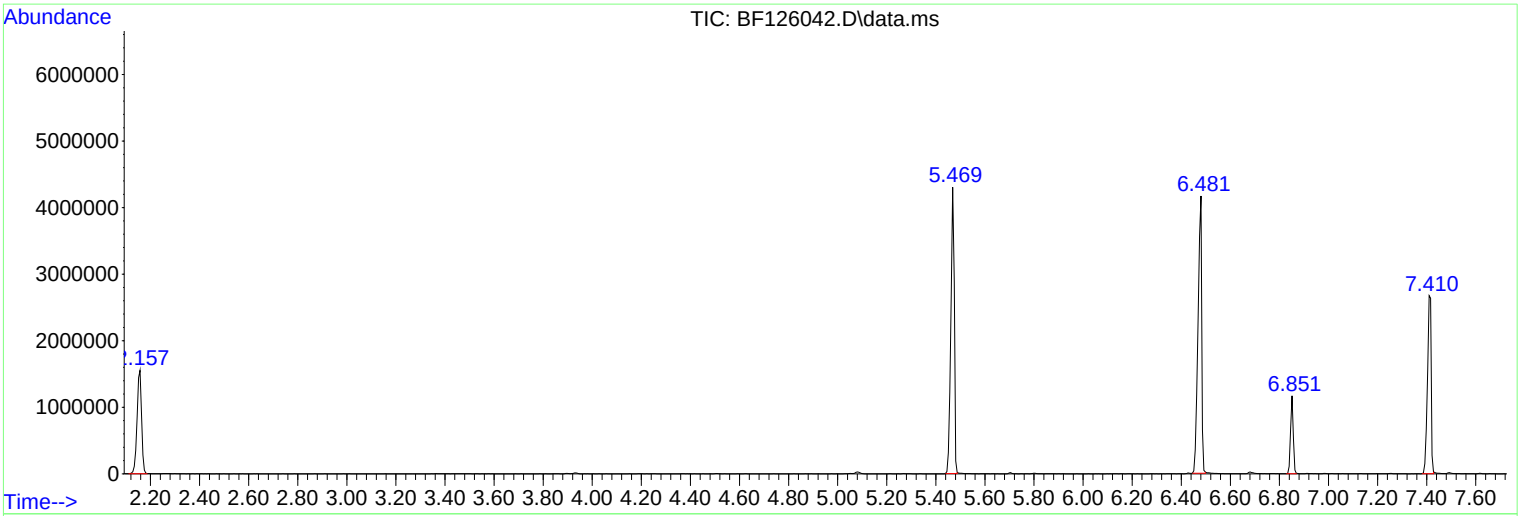
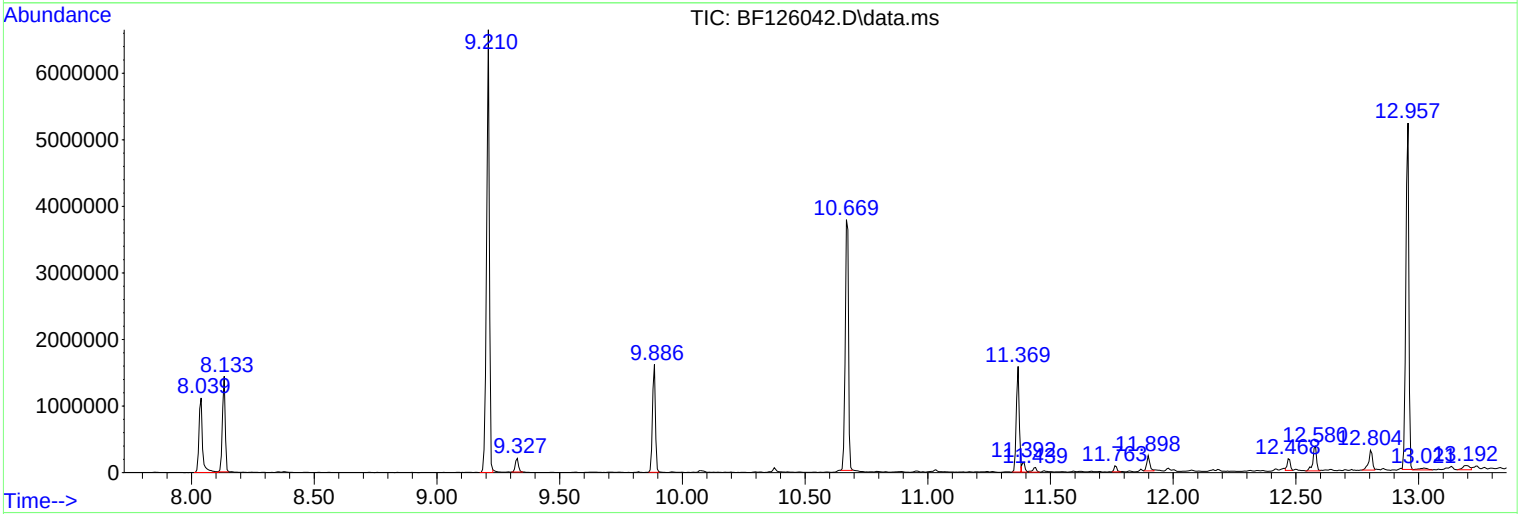
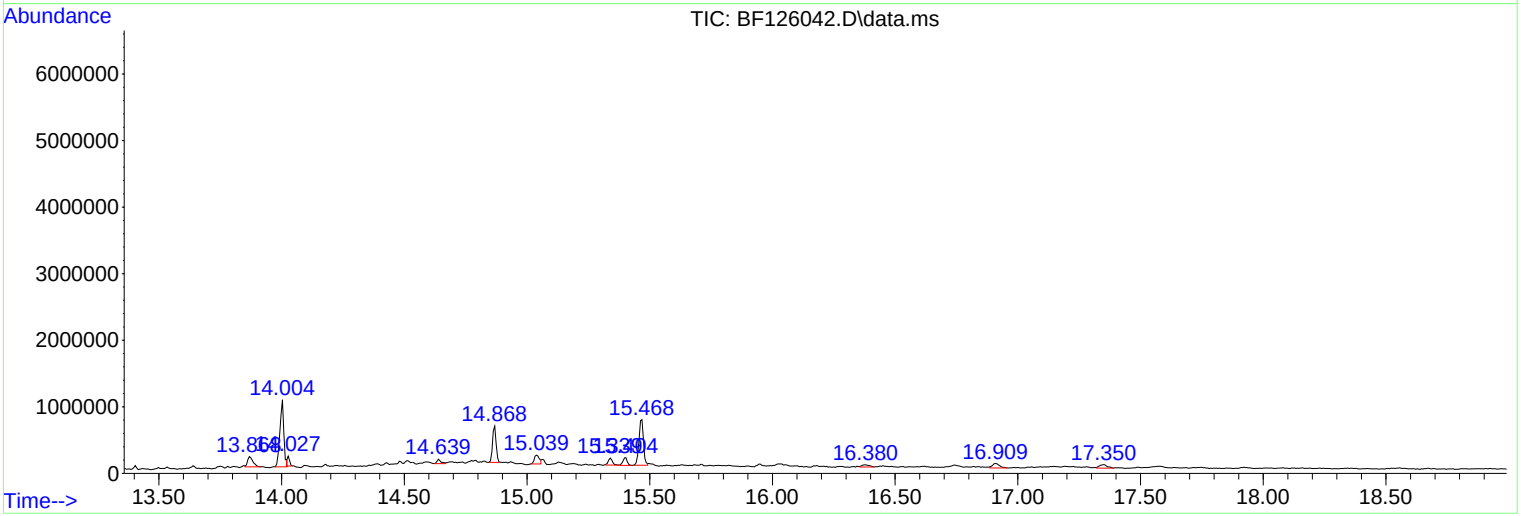
Instrument :
BNA_F
ClientSampleId :
VNJ-224

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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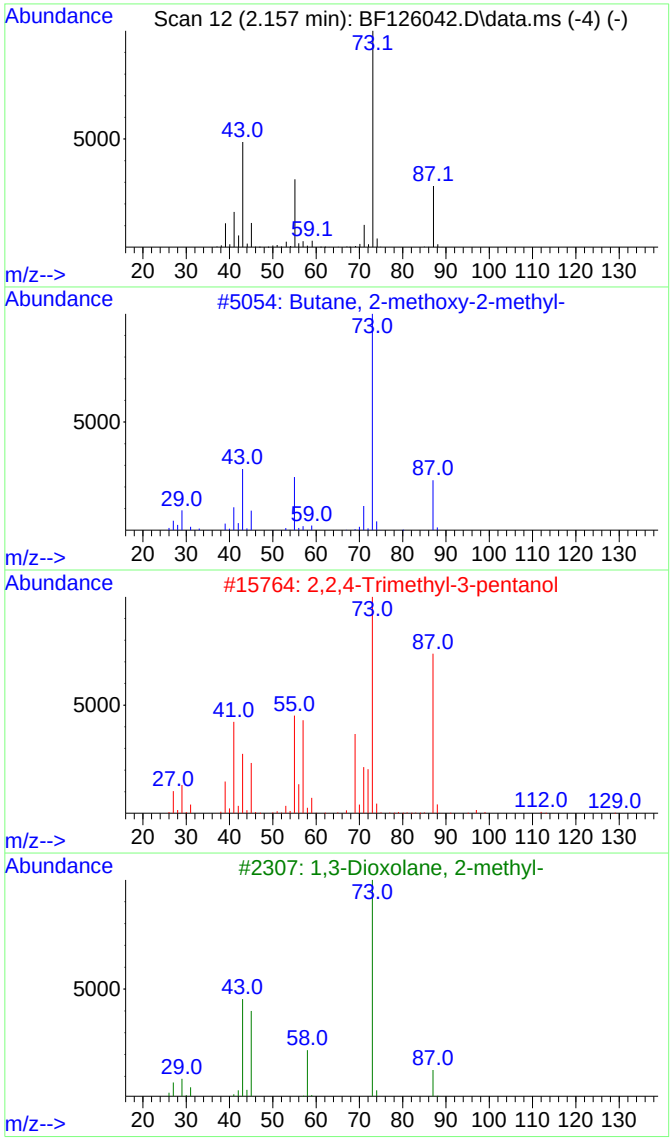
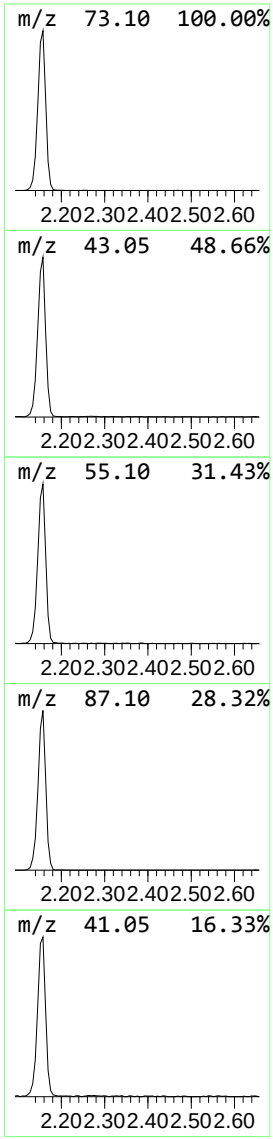
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	44.24 ng	1975540	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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
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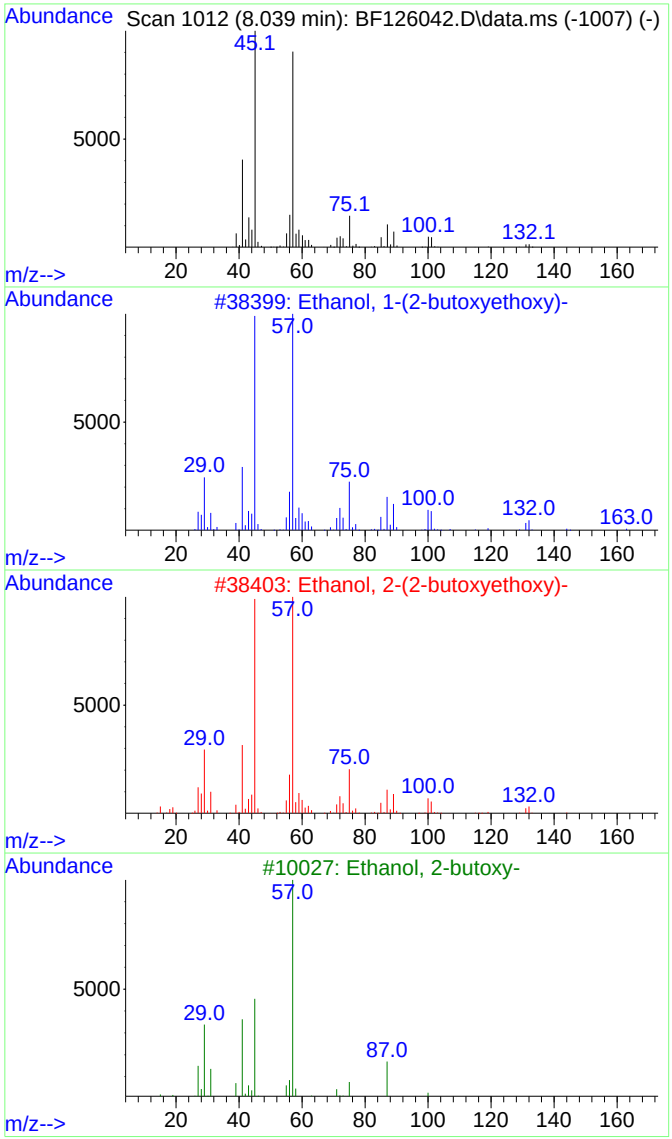
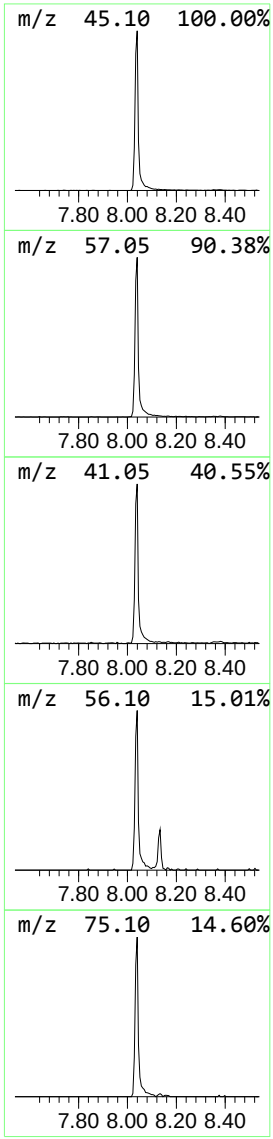
****
Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	19.95 ng	1123580	Naphthalene-d8	8.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50





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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

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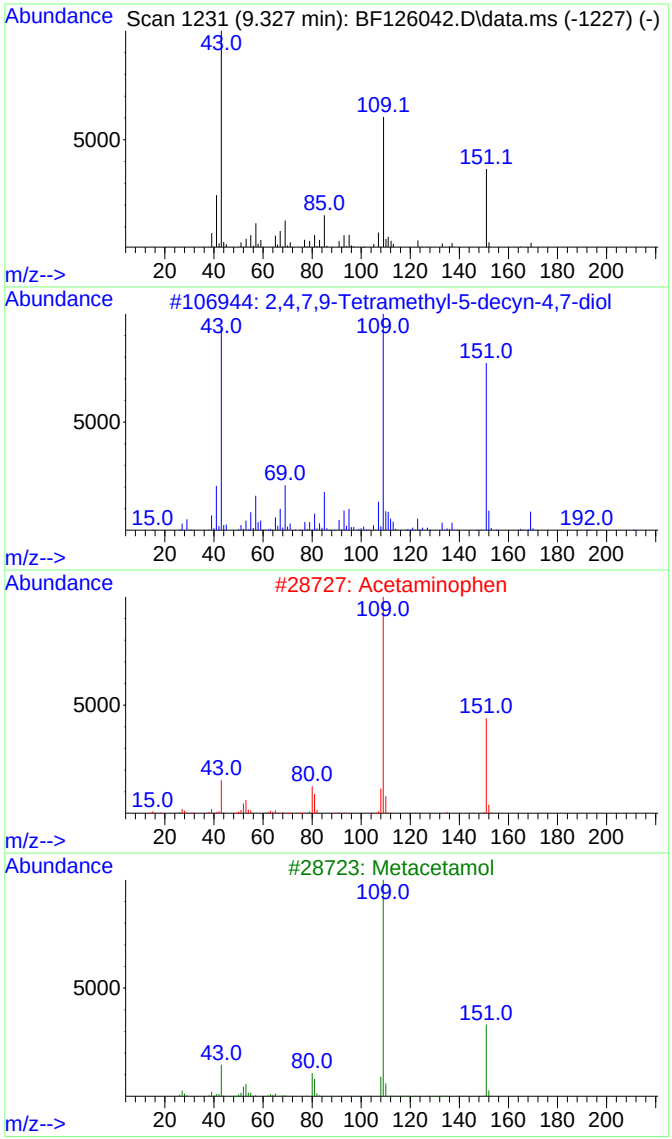
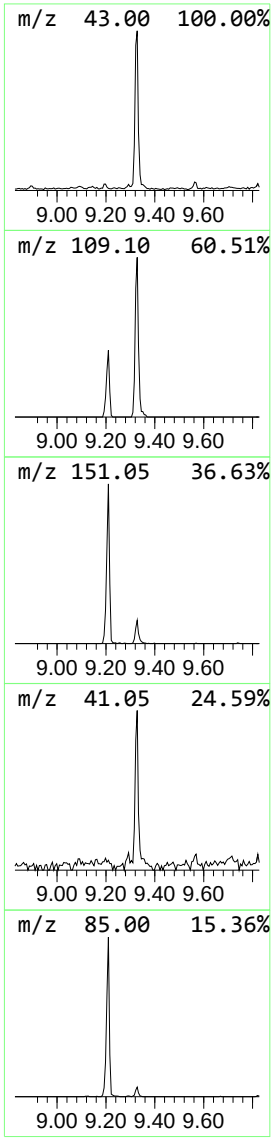
****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.327	2.73 ng	183210	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86
2	Acetaminophen	151	C8H9NO2	000103-90-2	49
3	Metacetamol	151	C8H9NO2	000621-42-1	47
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	38
5	benzenamine, 3-[(tetrahydro-2H-p...	193	C11H15NO2	1010400-28-1	38





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ClientSampleId :
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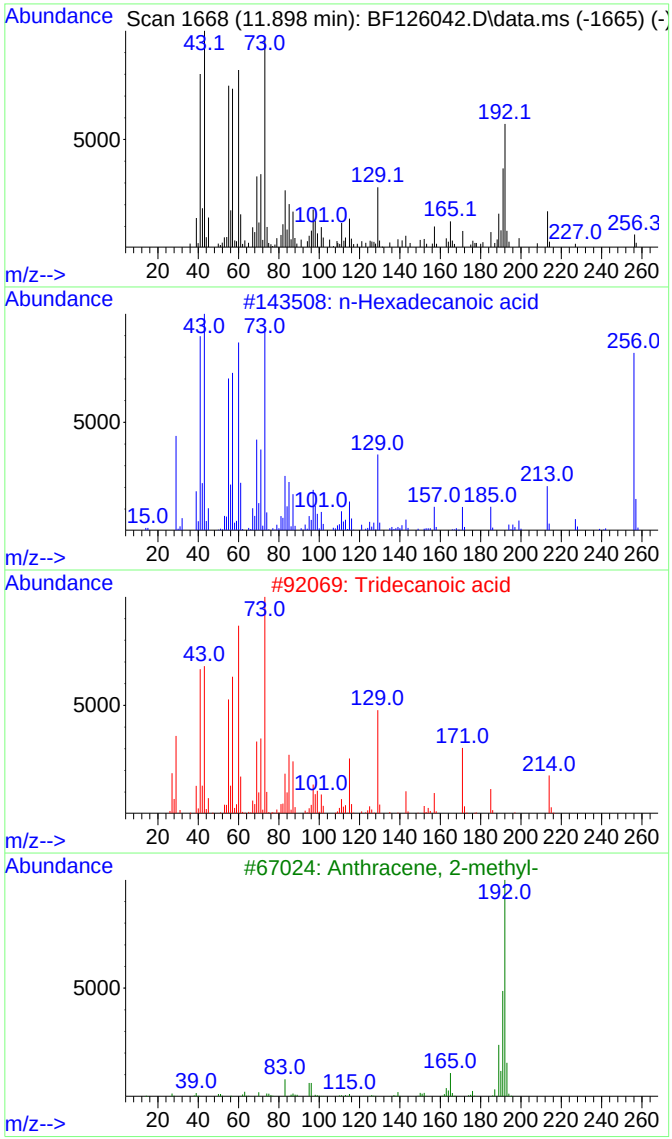
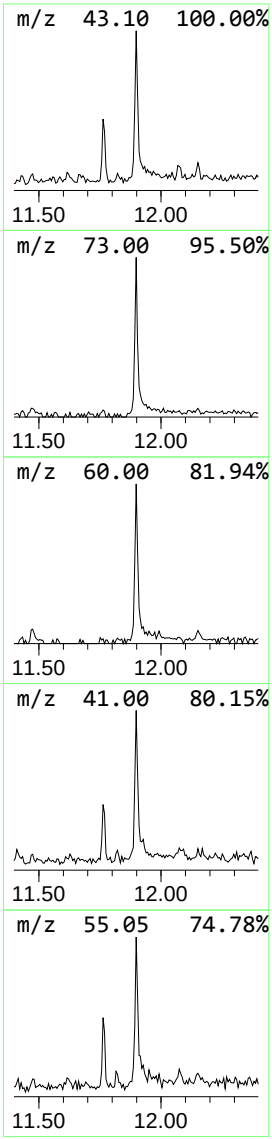
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	3.02 ng	199160	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	66
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	66
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Sample : M4448-01
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Instrument :
BNA_F
ClientSampleId :
VNJ-224

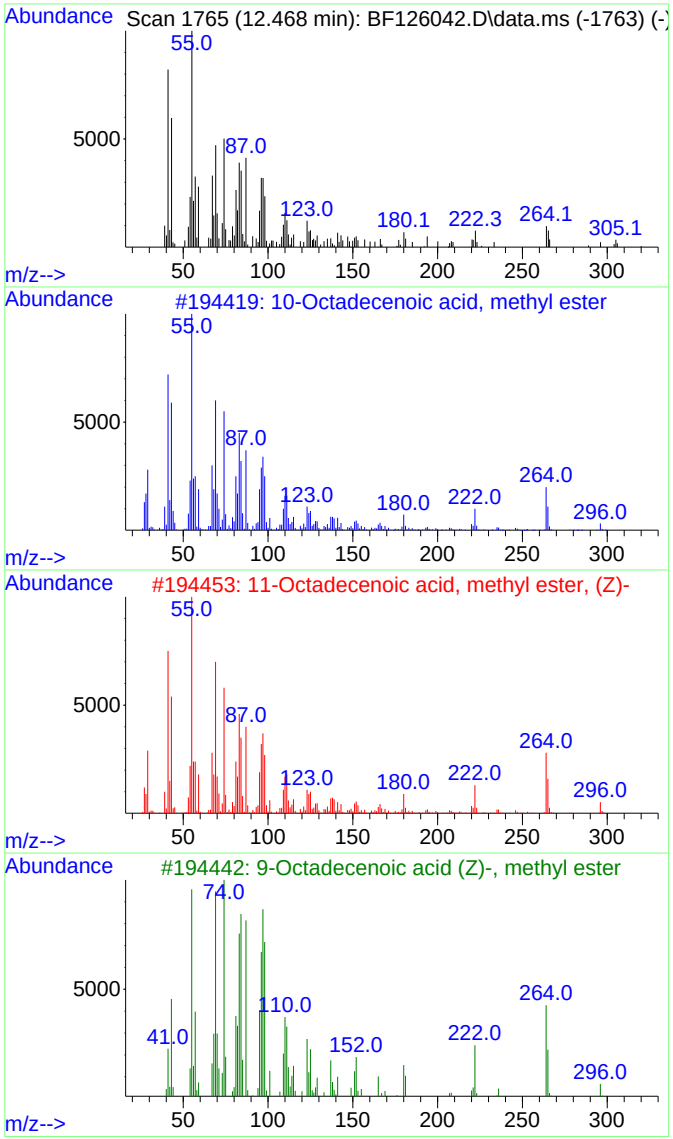
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

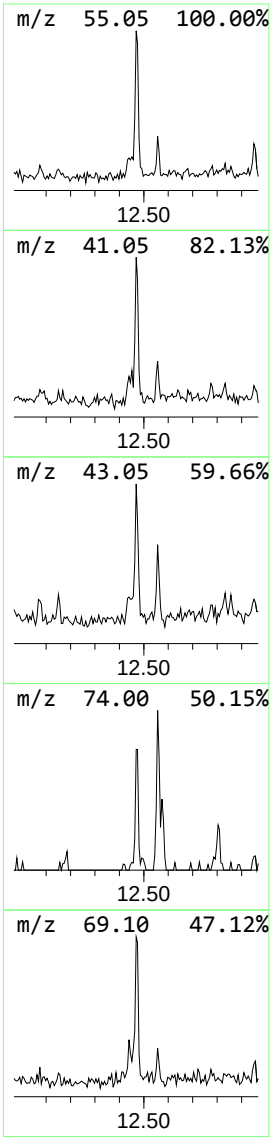
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.468	2.33 ng	153610	Phenanthrene-d10	11.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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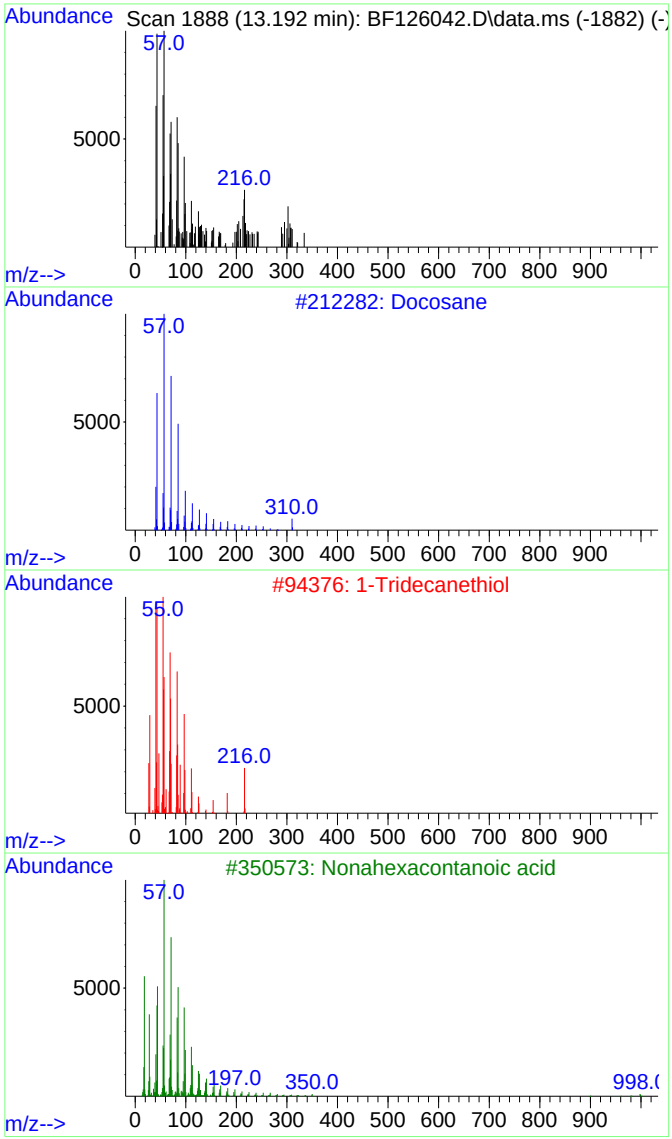
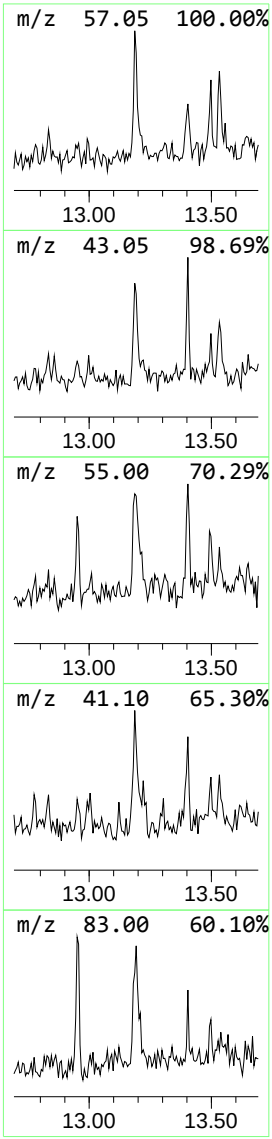
****

Peak Number 6 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	2.30 ng	128634	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	60
2	1-Tridecanethiol	216	C13H28S	019484-26-5	59
3	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	53
4	Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	49
5	Cyclohexadecane	224	C16H32	000295-65-8	47





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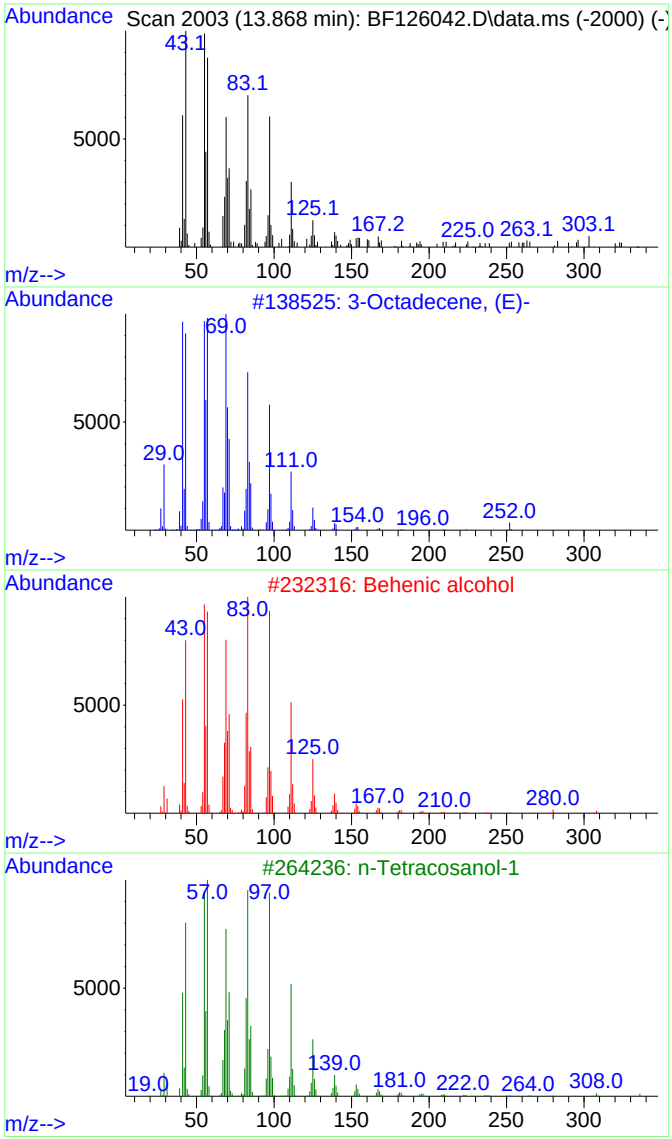
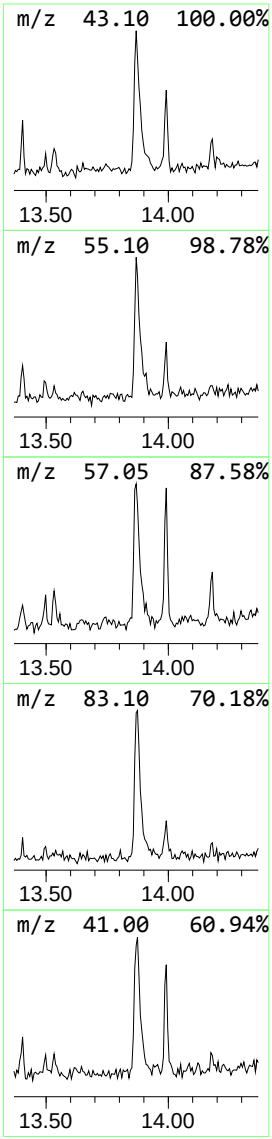
Peak Number 7 3-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	4.13 ng	230943	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	92
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Cycloeicosane	280	C20H40	000296-56-0	90





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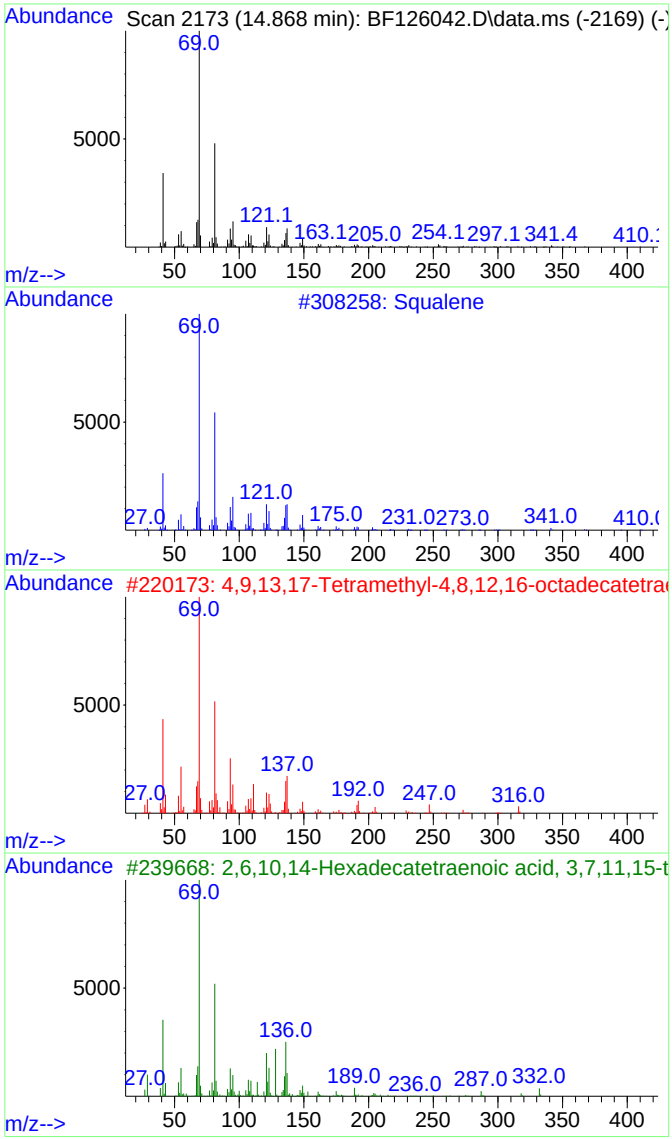
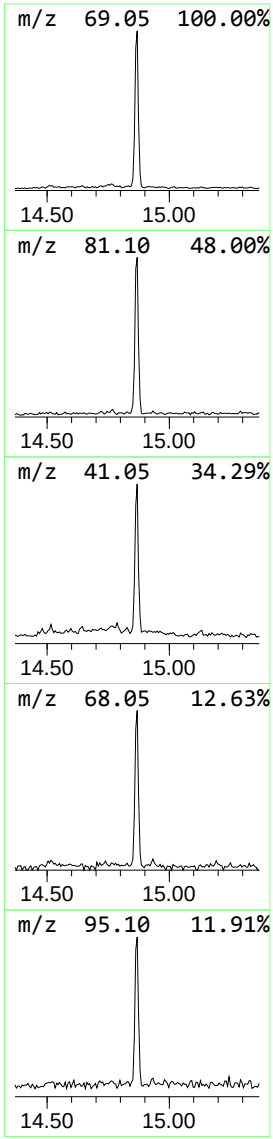
Peak Number 8 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	12.31 ng	540662	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64





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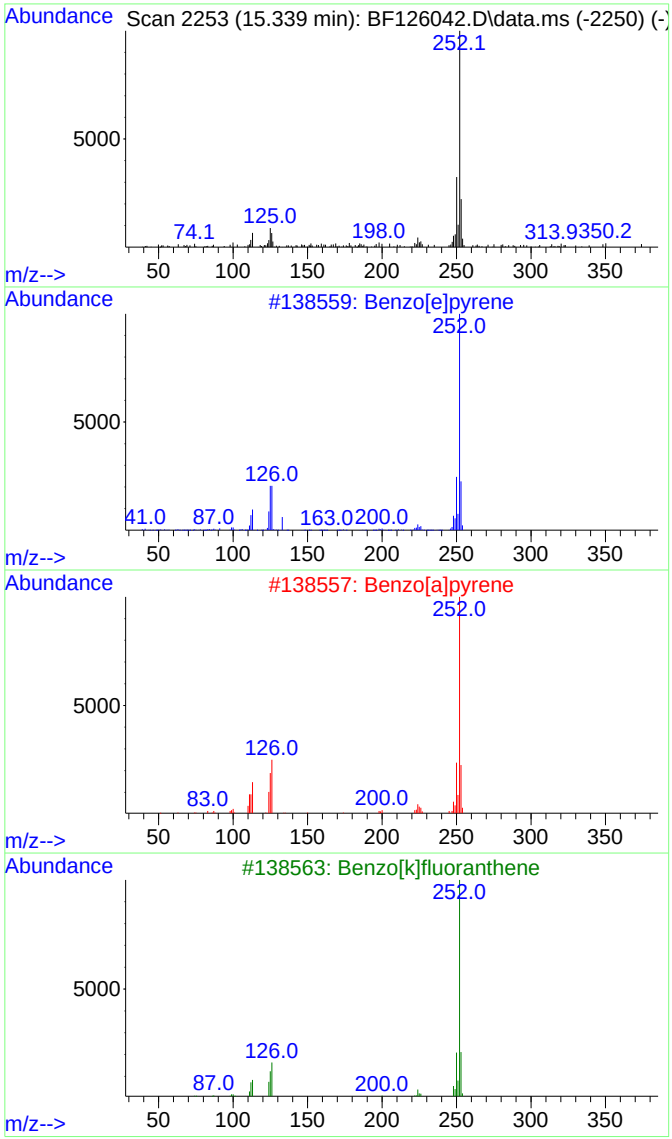
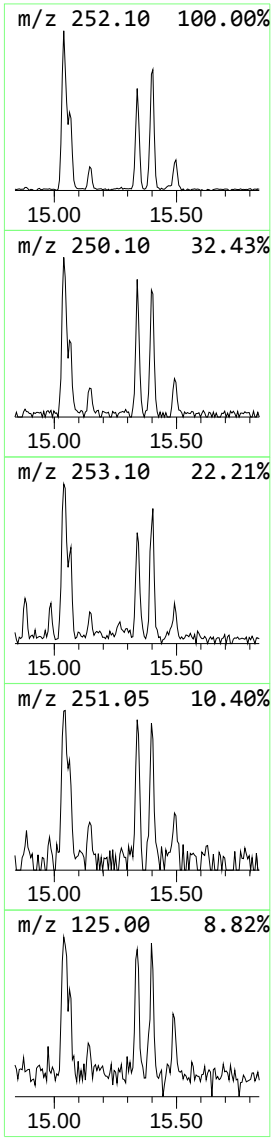
Peak Number 9 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	2.61 ng	114514	Perylene-d12	15.468

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126042.D
Acq On : 4 Nov 2021 13:17
Operator : JU/CG
Sample : M4448-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-224

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...	2.157	44.2	ng	1975540	1	6.851	893008	20.0
Ethanol, 1-(2-b...	8.039	19.9	ng	1123580	2	8.133	1126130	20.0
2,4,7,9-Tetrame...	9.327	2.7	ng	183210	3	9.886	1342020	20.0
n-Hexadecanoic ...	11.898	3.0	ng	199160	4	11.368	1319210	20.0
10-Octadecenoic...	12.468	2.3	ng	153610	4	11.368	1319210	20.0
Docosane	13.192	2.3	ng	128634	5	14.004	1119200	20.0
3-Octadecene, (E)-	13.868	4.1	ng	230943	5	14.004	1119200	20.0
Squalene	14.868	12.3	ng	540662	6	15.468	878347	20.0
Benzo[e]pyrene	15.339	2.6	ng	114514	6	15.468	878347	20.0