LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

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-BF043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137777.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	52	57	63	rVB	333697	445358	8.21%	1.033%
2	3.693	270	273	292	rBV	60593	175184	3.23%	0.406%
3	5.681	606	611	614	rBV	4538968	4159149	76.65%	9.651%
4	6.669	773	779	782	rBV	4219973	4201891	77.44%	9.750%
5	7.057	841	845	848	rBV	1697805	1303226	24.02%	3.024%
6	7.616	935	940	943	rBV	3016285	2766397	50.98%	6.419%
7	8.228	1040	1044	1055	rBV	696762	613480	11.31%	1.423%
8	8.339	1059	1063	1066	rBV	2220044	1764813	32.53%	4.095%
9	8.639	1112	1114	1123	rVB	99418	110361	2.03%	0.256%
10	9.416	1241	1246	1249	rBV	6599650	5426005	100.00%	12.590%
11	10.104	1359	1363	1366	rVB	2422851	1941293	35.78%	4.504%
12	10.133	1366	1368	1372	rVB	124616	90903	1.68%	0.211%
13	10.186	1372	1377	1383	rBV	176702	235565	4.34%	0.547%
14	10.304	1394	1397	1400	rVB	75501	64640	1.19%	0.150%
15	10.651	1453	1456	1459	rBV	168095	132079	2.43%	0.306%
16	10.892	1493	1497	1500	rBV	3569200	3031141	55.86%	7.033%
17	11.598	1613	1617	1619	rBV	2053961	1774741	32.71%	4.118%
18	11.622	1619	1621	1624	rVV	974620	724864	13.36%	1.682%
19	11.669	1624	1629	1632	rVV	251584	233040	4.29%	0.541%
20	12.104	1699	1703	1705	rBV2	560759	502777	9.27%	1.167%
21	12.127	1705	1707	1712	rVB2	152419	139205	2.57%	0.323%
22	12.216	1718	1722	1724	rBV2	201240	204072	3.76%	0.474%
23	12.651	1792	1796	1798	rBV	67151	74156	1.37%	0.172%
24	12.816	1820	1824	1829	rBV	1161985	1016778	18.74%	2.359%
25	12.892	1832	1837	1842	rVV3	100420	129275	2.38%	0.300%
26	12.986	1848	1853	1857	rVB2	143788	151801	2.80%	0.352%
27	13.027	1857	1860	1861	rBV	175351	169591	3.13%	0.394%
28	13.045	1861	1863	1869	rVB	852400	784258	14.45%	1.820%
29	13.186	1879	1887	1890	rBV	4557993	4003134	73.78%	9.289%
30	13.257	1895	1899	1903	rBV3	52270	92882	1.71%	0.216%
31	13.374	1916	1919	1921	rVB	126044	110804	2.04%	0.257%
32	13.439	1927	1930	1933	rVB	131739	104309	1.92%	0.242%
33	13.480	1933	1937	1939	rBV2	71186	76326	1.41%	0.177%
34	14.092	2039	2041	2049	rVB3	95537	162916	3.00%	0.378%
35	14.245	2062	2067	2070	rBV2	1373925	1590095	29.31%	3.690%
36	14.274	2070	2072	2079	rVB	377230	333723	6.15%	0.774%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

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-BF043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.357	2083	2086	2088	rBV	80566	66601	1.23%	0.155%
38	14.386	2088	2091	2094	rBV	99156	93783	1.73%	0.218%
39	14.698	2141	2144	2147	rVB	129845	107404	1.98%	0.249%
40	14.739	2148	2151	2153	rBV3	65627	72120	1.33%	0.167%
41	15.198	2226	2229	2233	rVB	82353	87895	1.62%	0.204%
42	15.345	2250	2254	2257	rBV	344930	526699	9.71%	1.222%
43	15.410	2262	2265	2271	rVB2	148883	187445	3.45%	0.435%
44	15.462	2271	2274	2277	rBV	73681	84911	1.56%	0.197%
45	15.680	2307	2311	2318	rVB	205217	287937	5.31%	0.668%
46	15.751	2319	2323	2330	rVV	336227	433013	7.98%	1.005%
47	15.821	2330	2335	2339	rVV	1064656	1465798	27.01%	3.401%
48	15.857	2339	2341	2347	rVB	150957	171319	3.16%	0.398%
49	16.321	2416	2420	2425	rVB2	134850	184874	3.41%	0.429%
50	17.451	2607	2612	2622	rVB2	141256	308125	5.68%	0.715%
51	17.951	2692	2697	2704	rBV	88456	178725	3.29%	0.415%

Sum of corrected areas: 43096881

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
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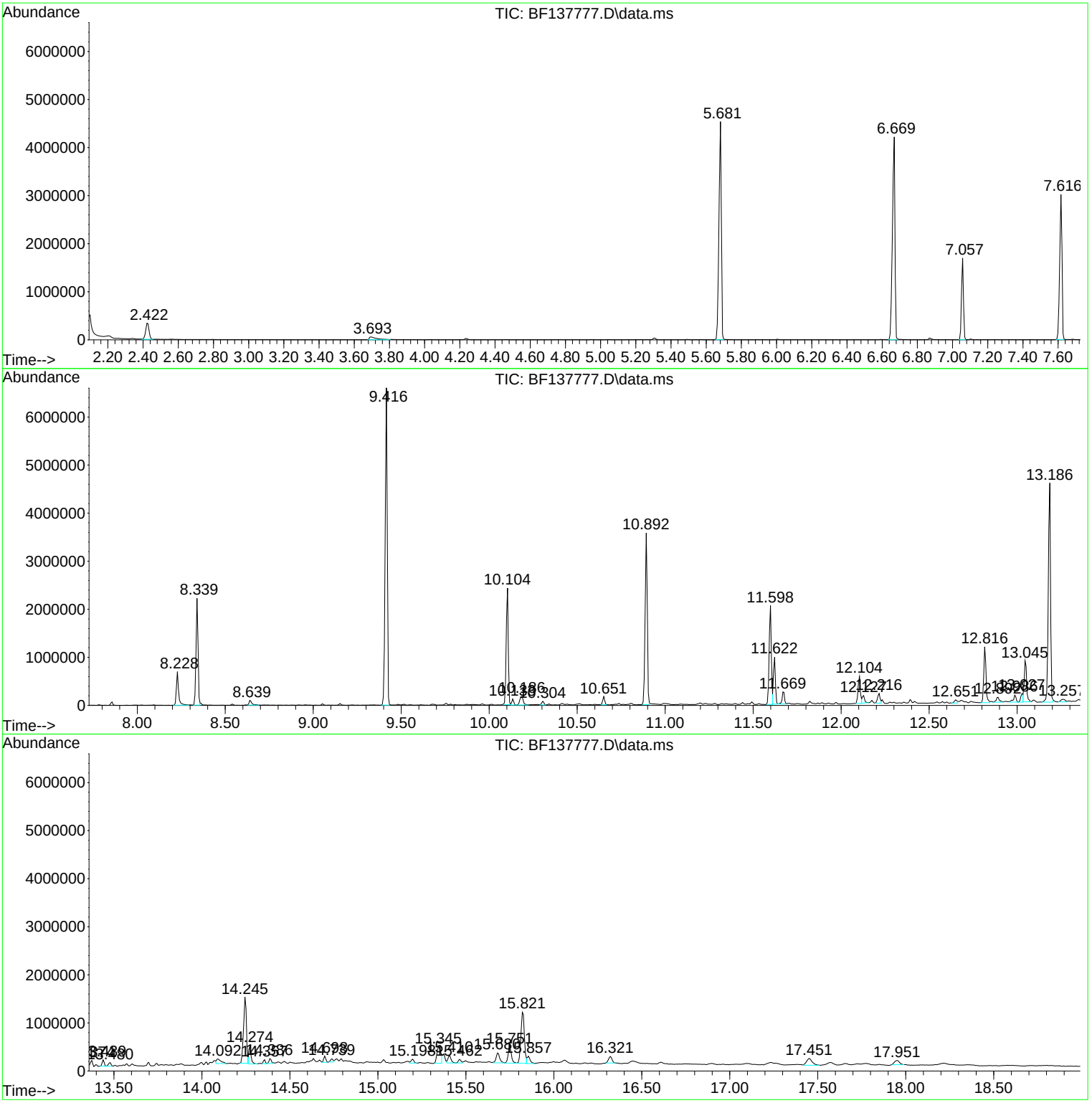
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

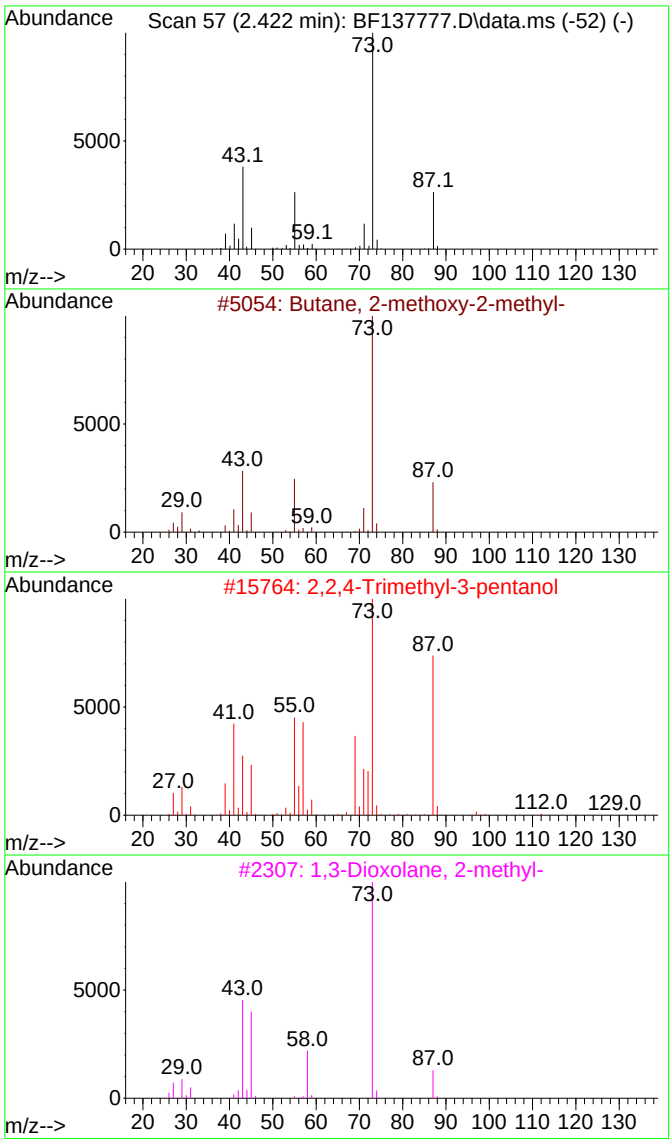
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

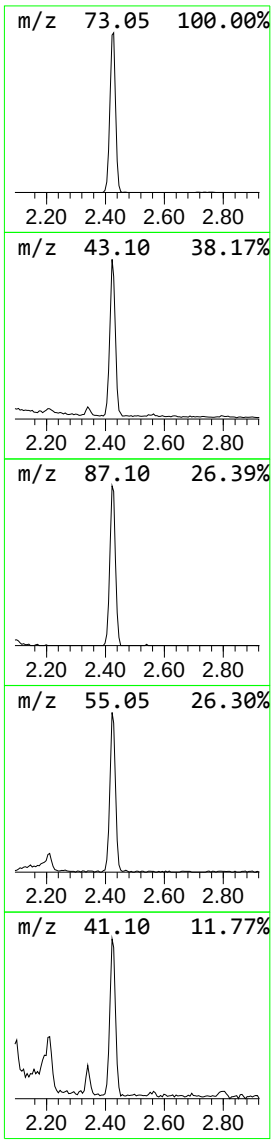
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.422	6.83 ng	445358	1,4-Dichlorobenzene-d4	7.057

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

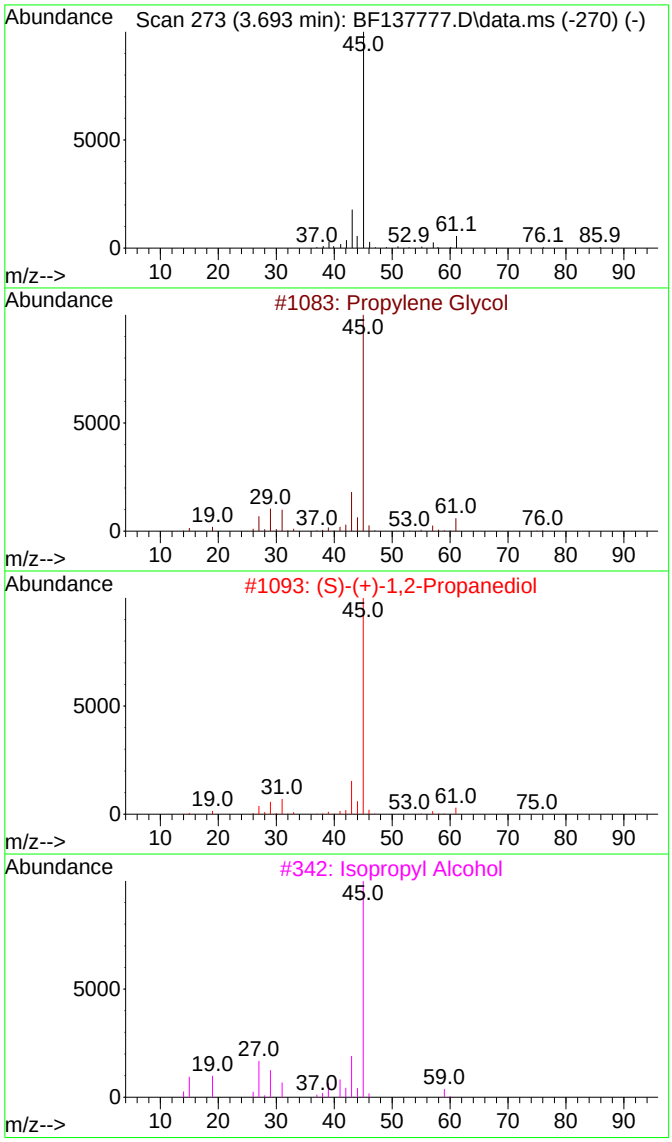
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

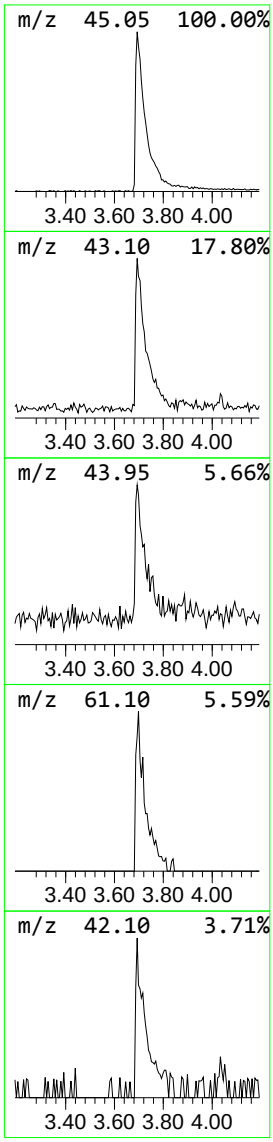
****

Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	2.69 ng	175184	1,4-Dichlorobenzene-d4	7.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

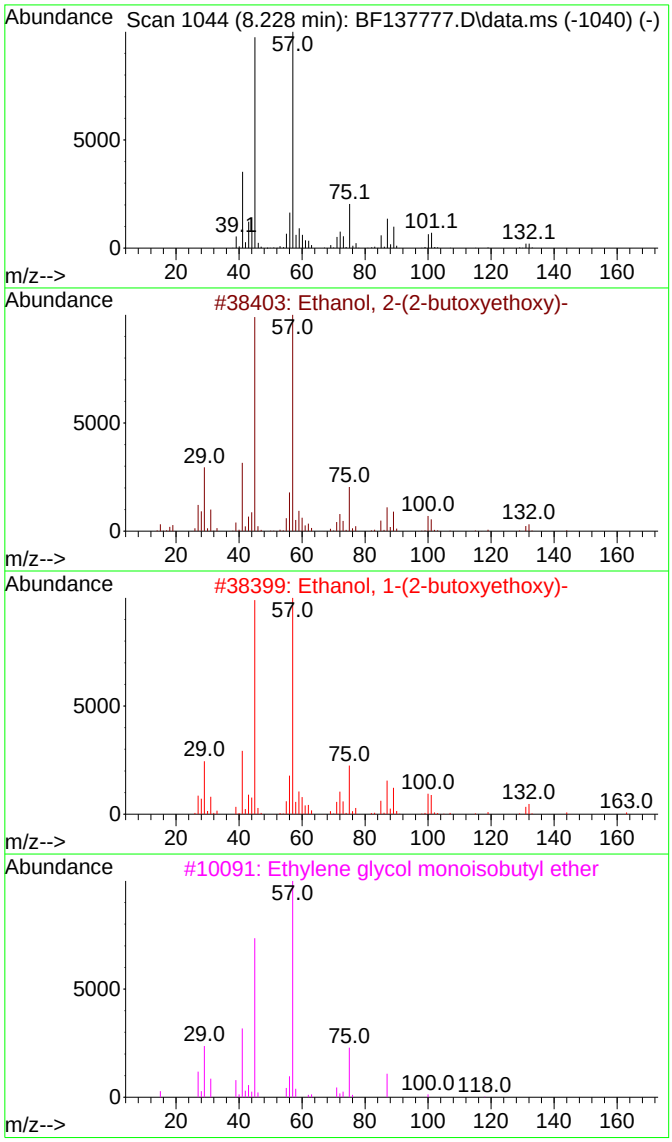
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

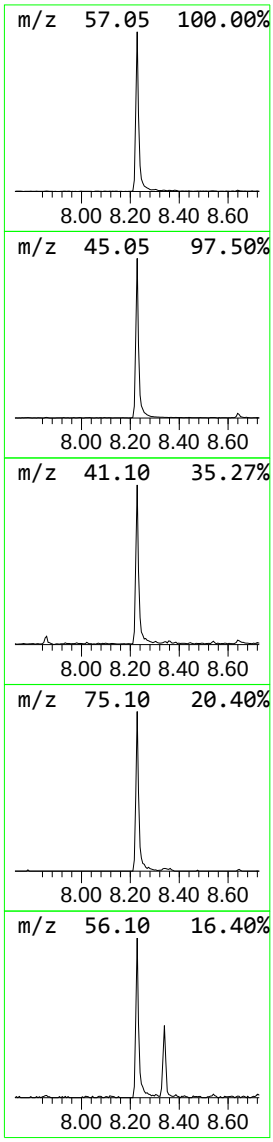
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.228	6.95 ng	613480	Naphthalene-d8	8.339

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	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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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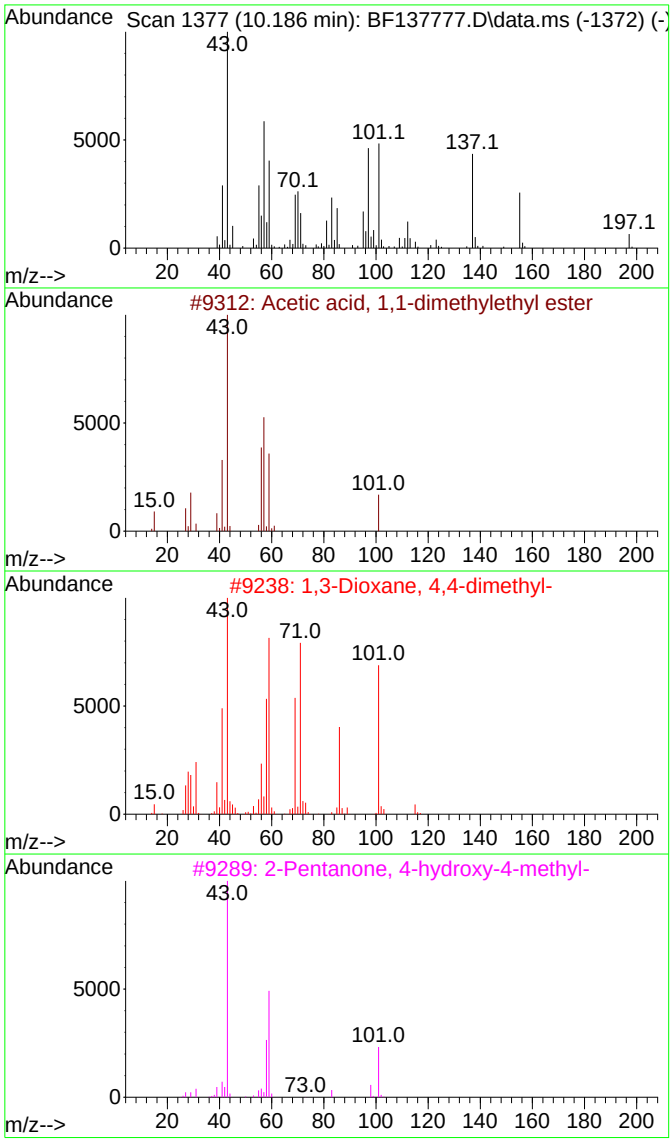
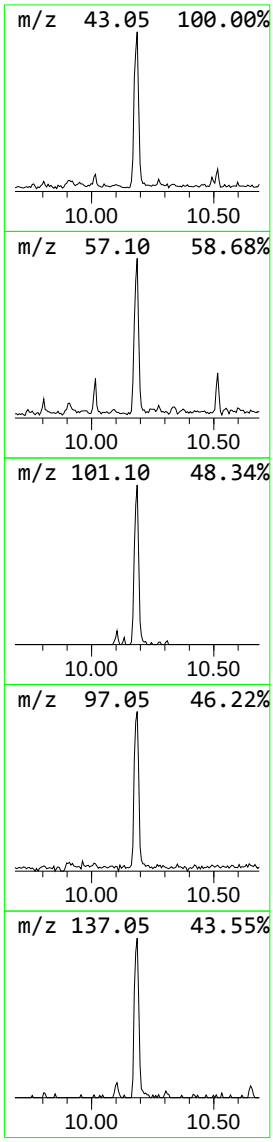
Peak Number 4 unknown10.186 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	2.43 ng	235565	Acenaphthene-d10	10.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	14
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
4	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
5	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

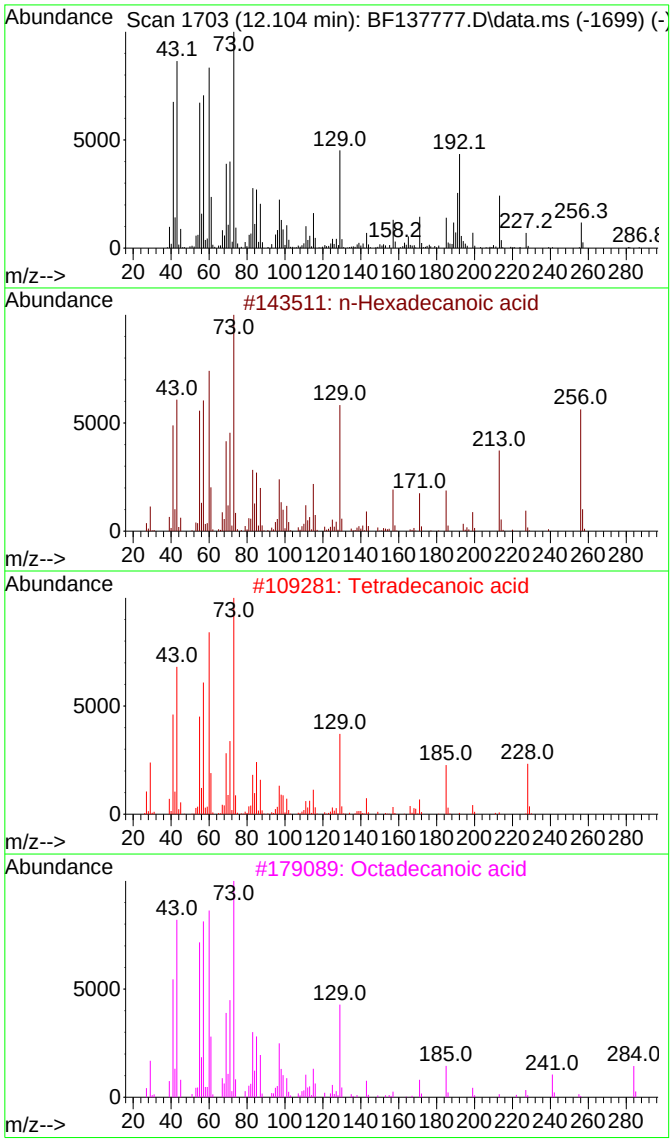
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

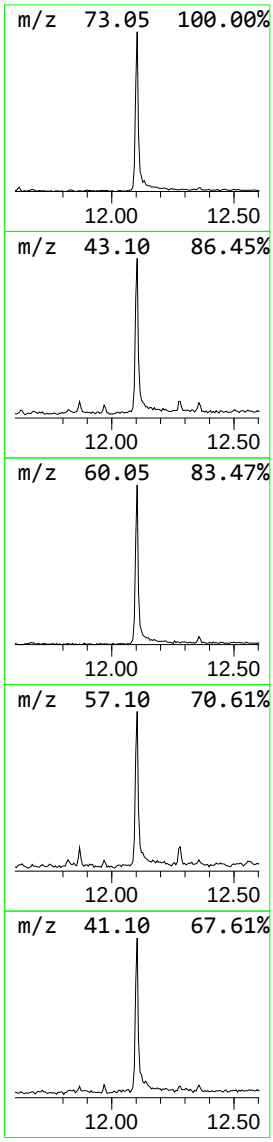
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	5.67 ng	502777	Phenanthrene-d10	11.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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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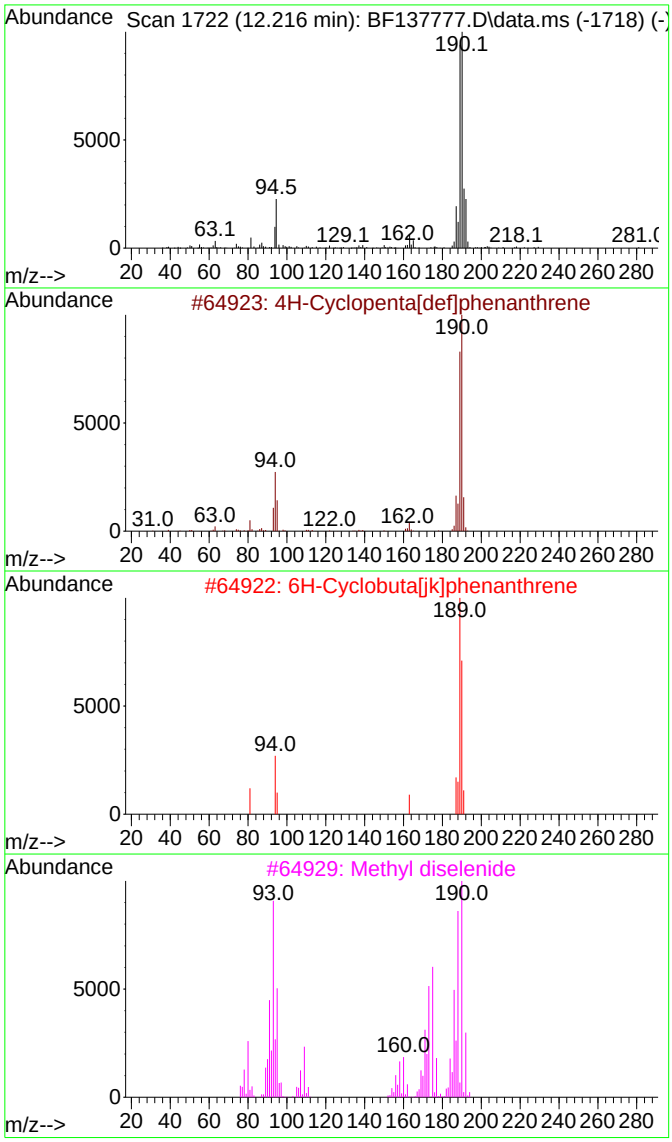
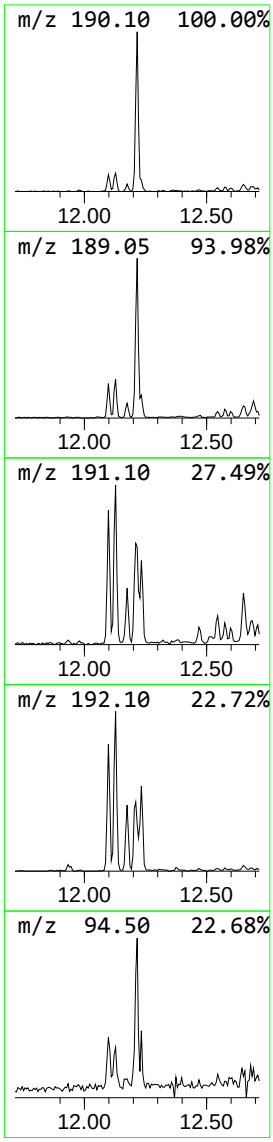
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.216	2.30 ng	204072	Phenanthrene-d10	11.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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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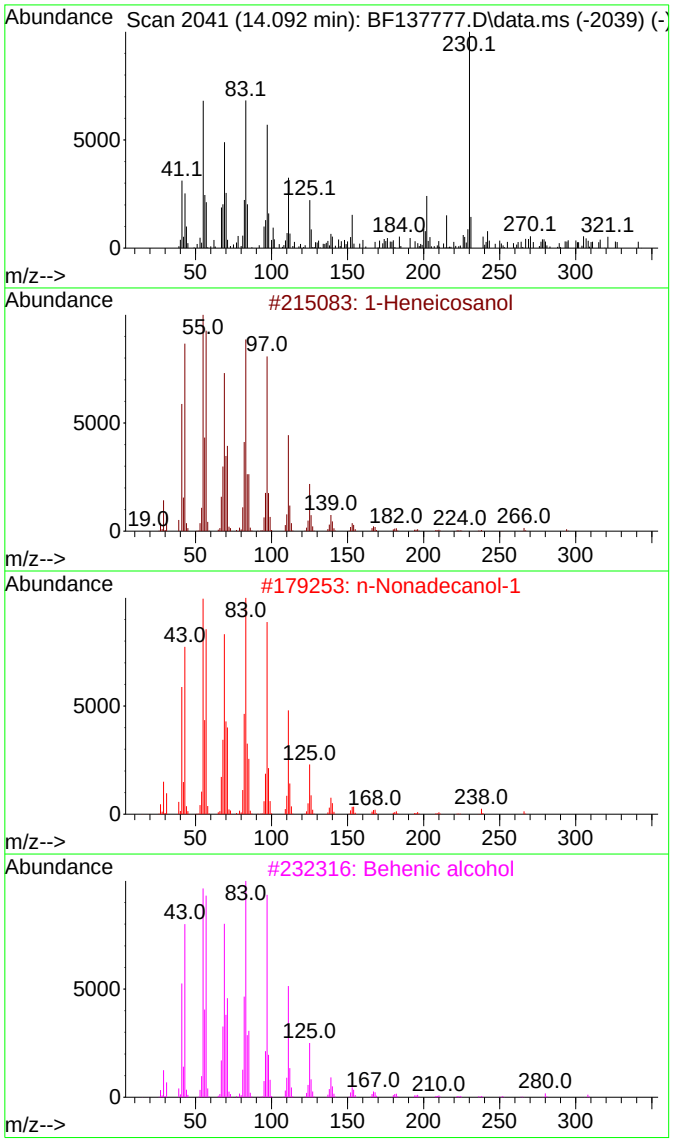
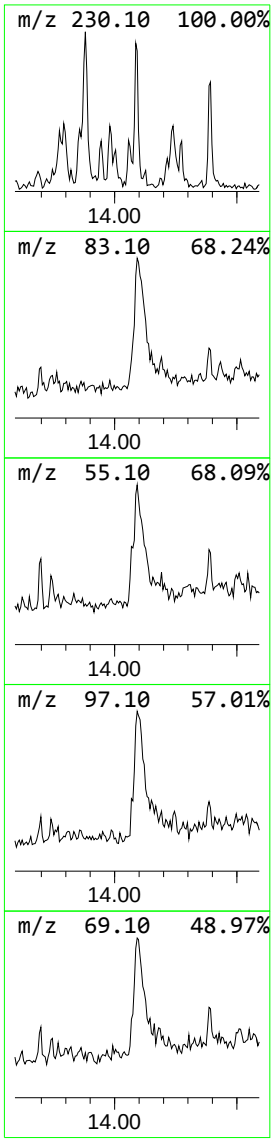
Peak Number 7 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	2.05 ng	162916	Chrysene-d12	14.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	50
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	45
3	Behenic alcohol	326	C22H46O	000661-19-8	45
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	43
5	Cycloeicosane	280	C20H40	000296-56-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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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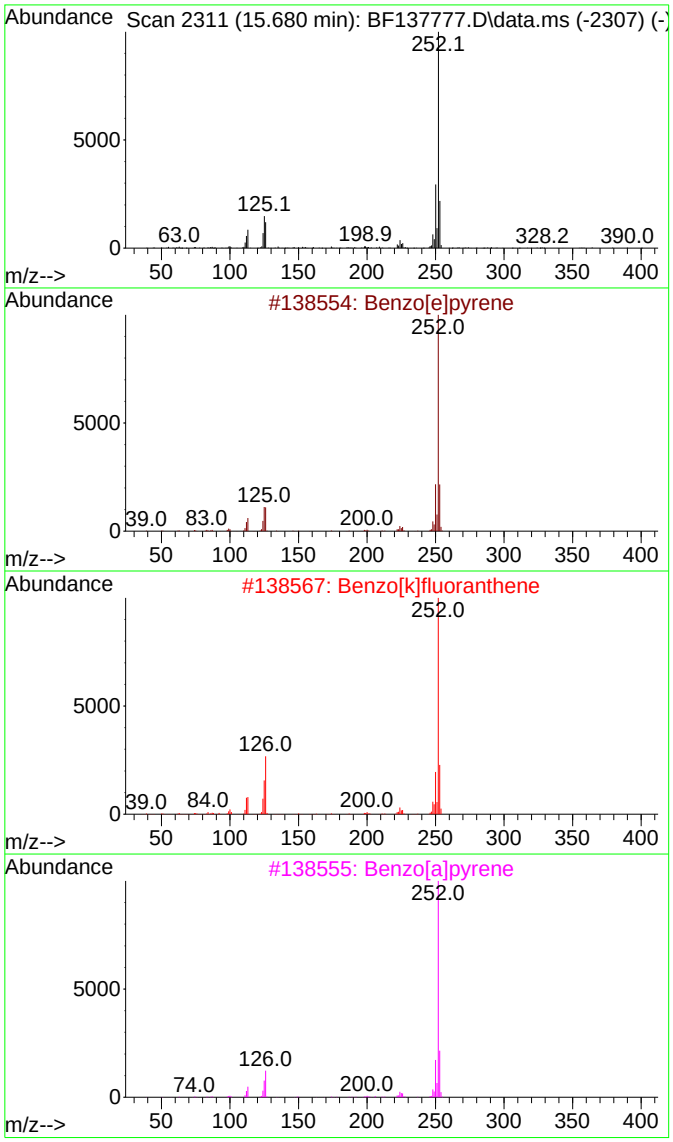
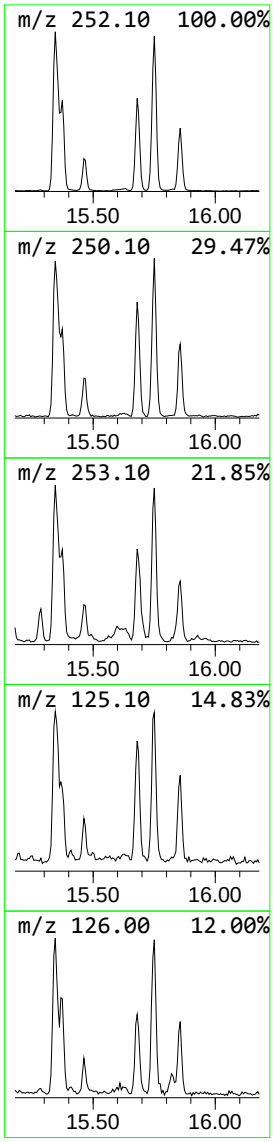
Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	3.93 ng	287937	Perylene-d12	15.821

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

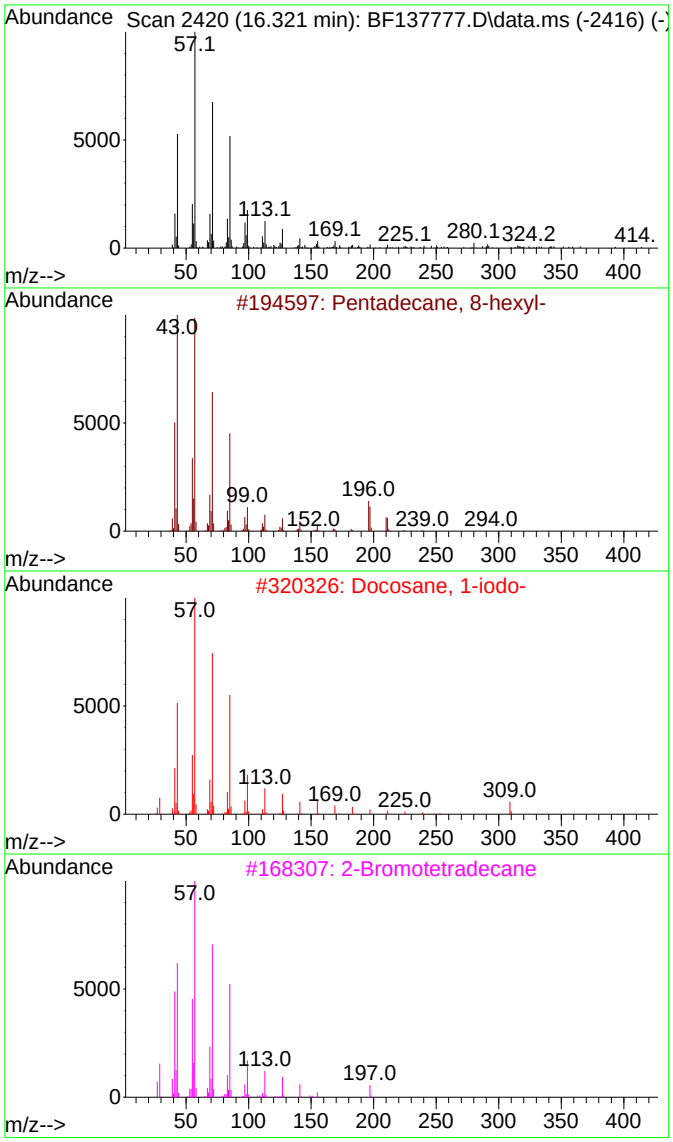
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

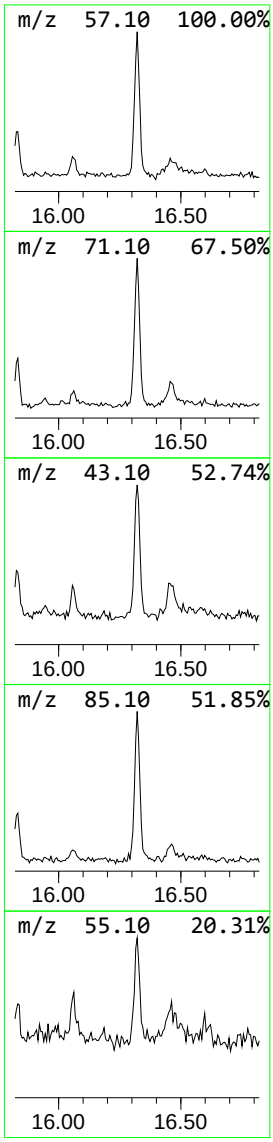
****

Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.321	2.52 ng	184874	Perylene-d12	15.821

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF043024\
Data File : BF137777.D
Acq On : 30 Apr 2024 18:31
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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...	2.422	6.8	ng	445358	1	7.057	1303230	20.0
Propylene Glycol	3.693	2.7	ng	175184	1	7.057	1303230	20.0
Ethanol, 2-(2-b...	8.228	7.0	ng	613480	2	8.339	1764810	20.0
unknown10.186	10.186	2.4	ng	235565	3	10.104	1941290	20.0
n-Hexadecanoic ...	12.104	5.7	ng	502777	4	11.598	1774740	20.0
4H-Cyclopenta[d...	12.216	2.3	ng	204072	4	11.598	1774740	20.0
1-Heneicosanol	14.092	2.0	ng	162916	5	14.245	1590100	20.0
Benzo[e]pyrene	15.680	3.9	ng	287937	6	15.821	1465800	20.0
Pentadecane, 8-...	16.321	2.5	ng	184874	6	15.821	1465800	20.0