LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	6	18	26	rBV	545606	803480	78.05%	7.843%
2	3.346	211	214	223	rBV	39341	78730	7.65%	0.769%
3	3.651	260	266	273	rVB4	10986	20178	1.96%	0.197%
4	3.922	307	312	318	rBV	12025	16365	1.59%	0.160%
5	4.010	321	327	329	rBV	13319	15433	1.50%	0.151%
6	4.040	329	332	337	rVB3	12990	18679	1.81%	0.182%
7	4.204	357	360	371	rVB4	9106	16570	1.61%	0.162%
8	4.451	398	402	408	rBV	15600	18595	1.81%	0.182%
9	4.604	423	428	434	rBV	85842	98029	9.52%	0.957%
10	4.769	452	456	459	rBV	20984	24311	2.36%	0.237%
11	5.016	495	498	506	rVB	53198	60918	5.92%	0.595%
12	5.434	565	569	582	rBV	954836	948788	92.17%	9.261%
13	6.228	699	704	713	rBV3	7429	11586	1.13%	0.113%
14	6.434	735	739	755	rBV	986155	899998	87.43%	8.785%
15	6.622	766	771	778	rBV	18015	28385	2.76%	0.277%
16	6.781	795	798	803	rVB	345130	283751	27.56%	2.770%
17	6.863	808	812	816	rVV2	11204	14138	1.37%	0.138%
18	6.904	816	819	824	rVB2	11384	12128	1.18%	0.118%
19	7.345	890	894	897	rBV	690010	569848	55.36%	5.562%
20	7.598	934	937	942	rBV	28850	24405	2.37%	0.238%
21	8.057	1012	1015	1019	rBV	407533	337838	32.82%	3.298%
22	8.239	1040	1046	1051	rBV4	5788	12134	1.18%	0.118%
23	8.339	1059	1063	1065	rBV3	10558	12964	1.26%	0.127%
24	8.380	1065	1070	1072	rBV4	24447	33523	3.26%	0.327%
25	9.133	1194	1198	1202	rBV	1200226	1029405	100.00%	10.048%
26	9.680	1288	1291	1295	rBV	18599	17621	1.71%	0.172%
27	9.769	1303	1306	1311	rBV	82725	70335	6.83%	0.687%
28	9.816	1311	1314	1318	rVV	423824	336543	32.69%	3.285%
29	9.845	1318	1319	1324	rVV	15683	14697	1.43%	0.143%
30	9.916	1326	1331	1340	rVB2	149144	211988	20.59%	2.069%
31	10.369	1404	1408	1413	rVB	12343	12265	1.19%	0.120%
32	10.610	1446	1449	1458	rBV	534178	516604	50.18%	5.043%
33	10.704	1458	1465	1466	rVV2	13337	25402	2.47%	0.248%
34	10.733	1466	1470	1478	rVB	279475	270137	26.24%	2.637%
35	11.204	1546	1550	1556	rVB2	9023	13420	1.30%	0.131%
36	11.310	1564	1568	1571	rBV	379421	323314	31.41%	3.156%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.333	1571	1572	1575	rVV	79902	47379	4.60%	0.462%
38	11.386	1578	1581	1584	rVB	26859	24184	2.35%	0.236%
39	11.704	1633	1635	1637	rBV	21941	14863	1.44%	0.145%
40	11.845	1656	1659	1665	rBV2	70896	78280	7.60%	0.764%
41	11.927	1670	1673	1676	rBV2	22456	21711	2.11%	0.212%
42	12.368	1744	1748	1750	rBV	13064	13233	1.29%	0.129%
43	12.410	1750	1755	1760	rVB5	16436	28395	2.76%	0.277%
44	12.533	1772	1776	1779	rBV	142436	120241	11.68%	1.174%
45	12.633	1790	1793	1796	rBV3	12254	14661	1.42%	0.143%
46	12.763	1809	1815	1821	rBV	137194	142164	13.81%	1.388%
47	12.904	1833	1839	1843	rBV	1018365	904964	87.91%	8.834%
48	12.980	1849	1852	1858	rBV6	10866	17493	1.70%	0.171%
49	13.068	1863	1867	1869	rBV4	12565	15694	1.52%	0.153%
50	13.092	1869	1871	1875	rVB	24728	21815	2.12%	0.213%
51	13.163	1880	1883	1885	rBV	14176	12855	1.25%	0.125%
52	13.198	1886	1889	1892	rVB2	17009	14323	1.39%	0.140%
53	13.321	1907	1910	1917	rBV	12404	13766	1.34%	0.134%
54	13.745	1980	1982	1984	rVB	14320	11485	1.12%	0.112%
55	13.768	1984	1986	1990	rBV2	10579	17378	1.69%	0.170%
56	13.810	1991	1993	1998	rVB4	11950	13933	1.35%	0.136%
57	13.868	1998	2003	2005	rBV5	18407	31537	3.06%	0.308%
58	13.968	2013	2020	2023	rBV2	395558	446332	43.36%	4.357%
59	13.998	2023	2025	2029	rVV	72669	67619	6.57%	0.660%
60	14.074	2033	2038	2040	rBV3	18534	24737	2.40%	0.241%
61	14.127	2044	2047	2050	rBV3	18640	21034	2.04%	0.205%
62	14.362	2084	2087	2089	rVB	21593	19795	1.92%	0.193%
63	14.433	2096	2099	2102	rBV4	22368	27803	2.70%	0.271%
64	14.751	2150	2153	2155	rBV4	10475	12405	1.21%	0.121%
65	14.815	2162	2164	2167	rBV	17550	18188	1.77%	0.178%
66	15.021	2195	2199	2203	rBV	84482	138539	13.46%	1.352%
67	15.133	2215	2218	2222	rBV	17103	22049	2.14%	0.215%
68	15.333	2248	2252	2256	rBV	50982	62319	6.05%	0.608%
69	15.398	2259	2263	2268	rBV	76466	103821	10.09%	1.013%
70	15.462	2269	2274	2278	rBV	303477	387217	37.62%	3.780%
71	16.980	2527	2532	2541	rVB2	36990	77974	7.57%	0.761%
72	17.439	2607	2610	2616	rVB3	18087	31820	3.09%	0.311%

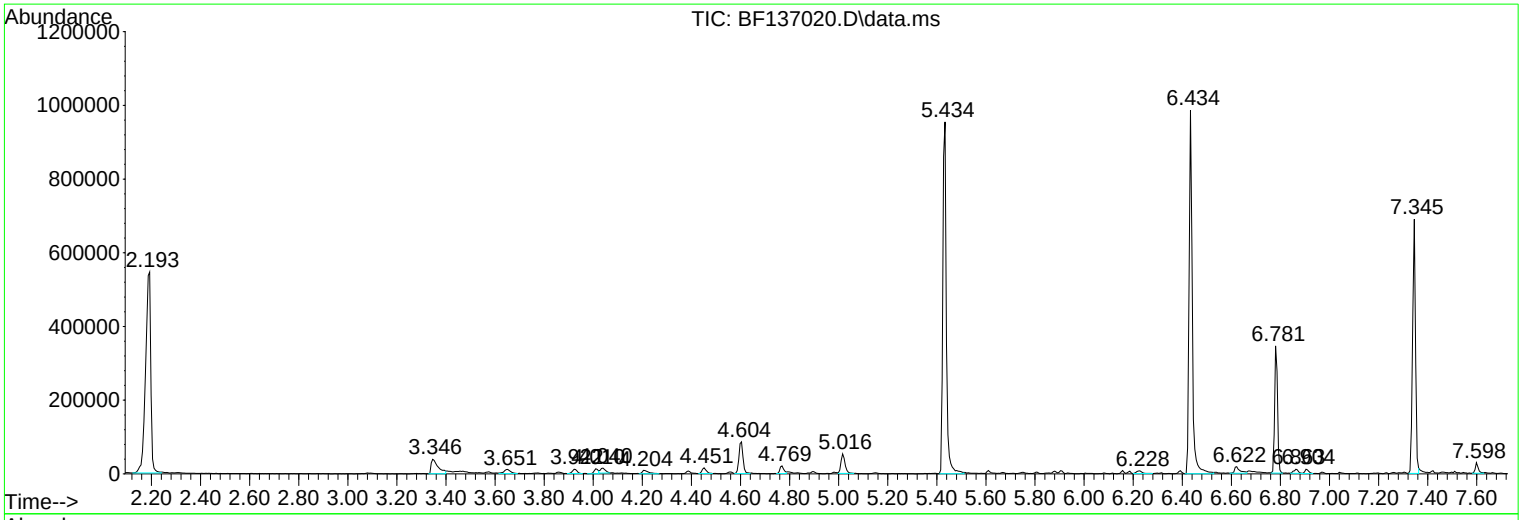
Sum of corrected areas: 10244511

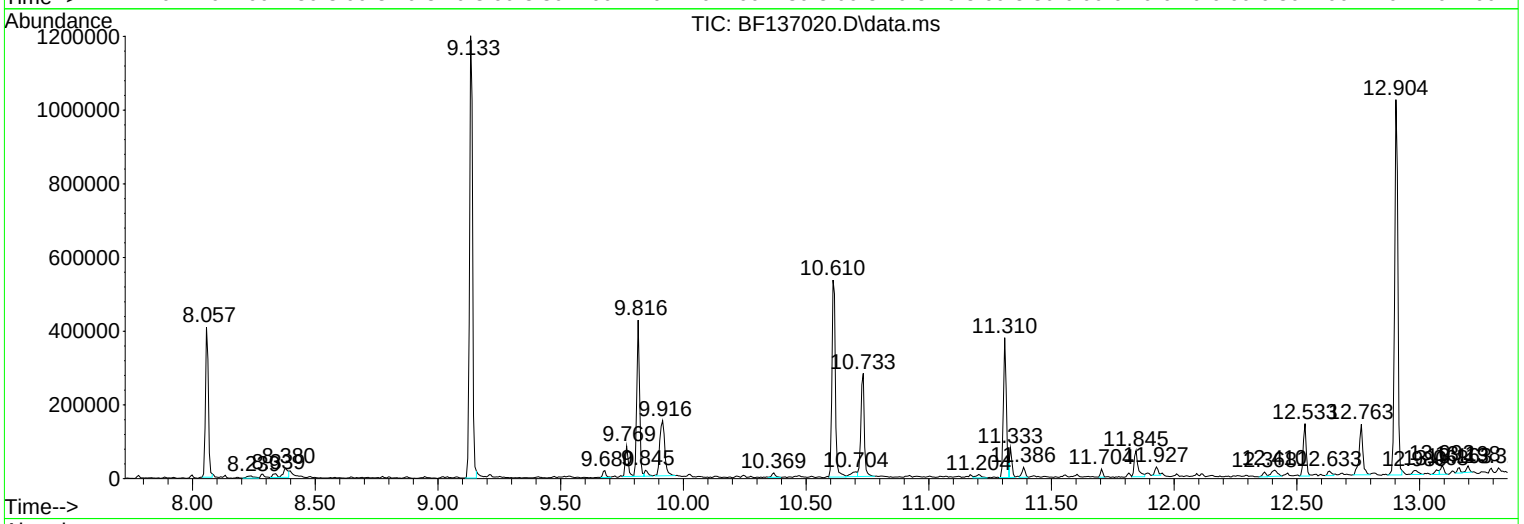
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

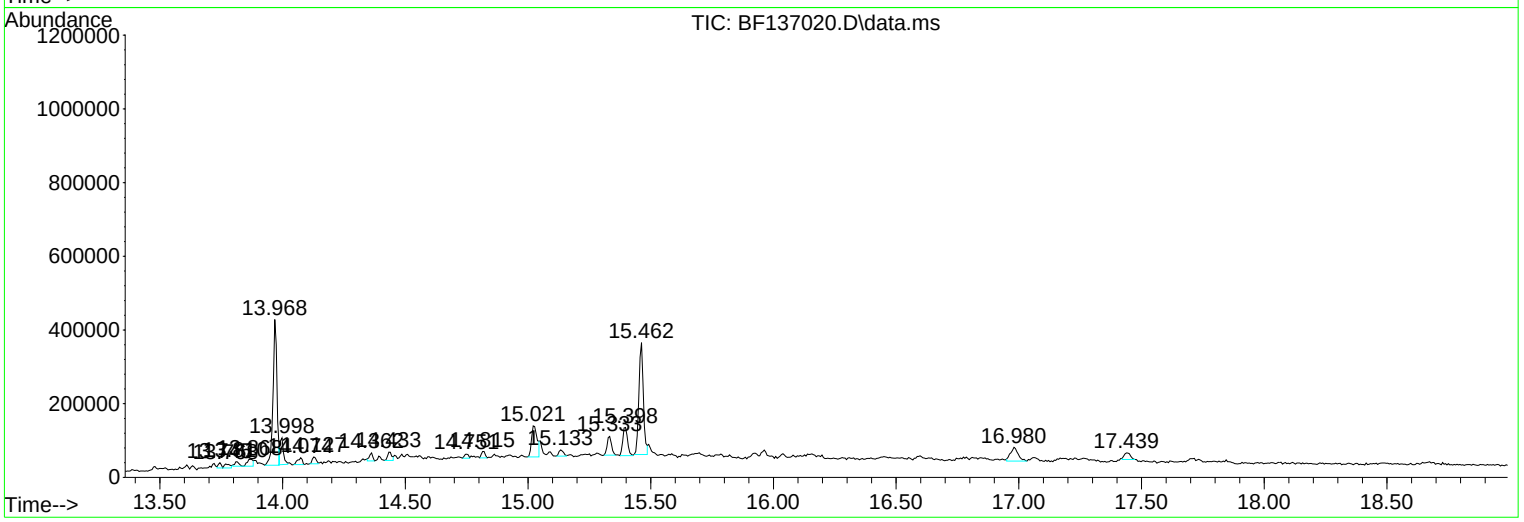
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

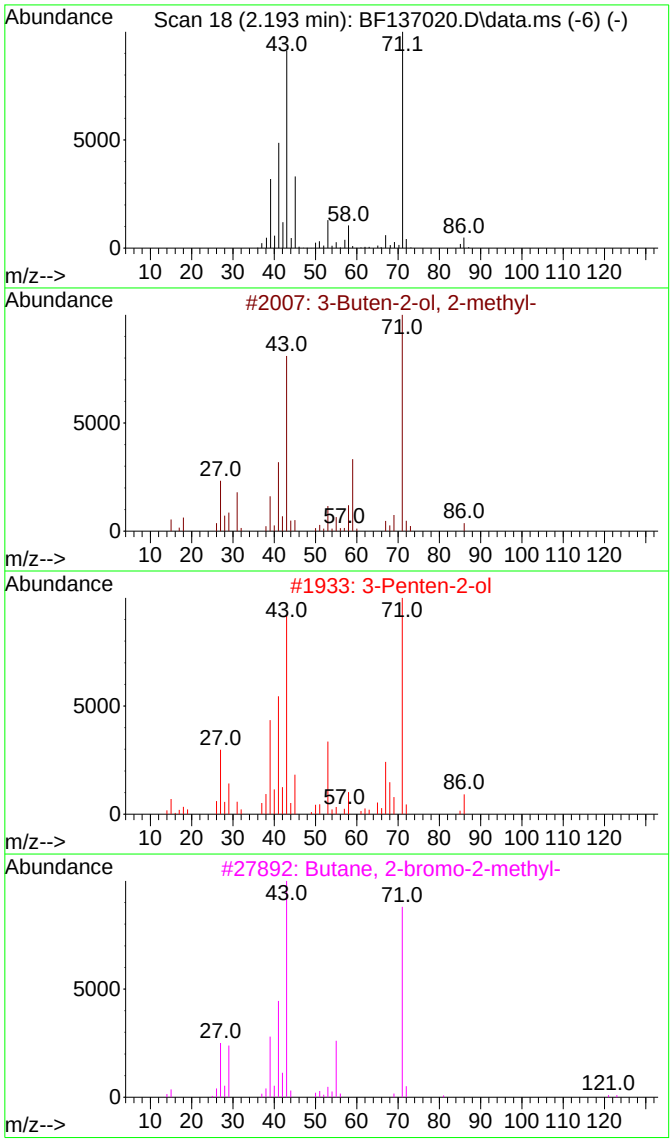
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

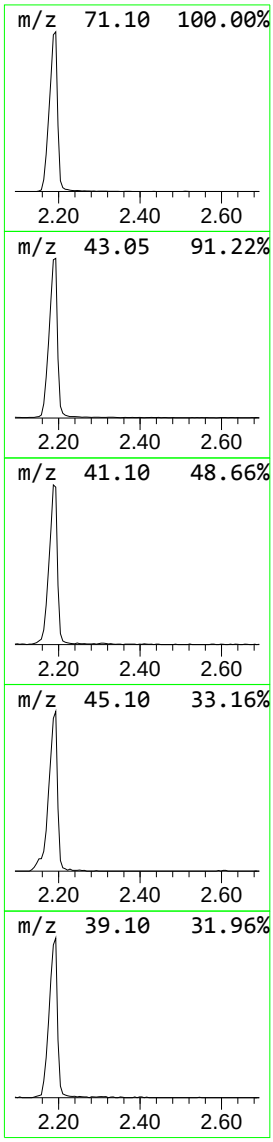
****

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	56.63 ng	803480	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2	3-Penten-2-ol	86	C5H10O	001569-50-2	64
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	50
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

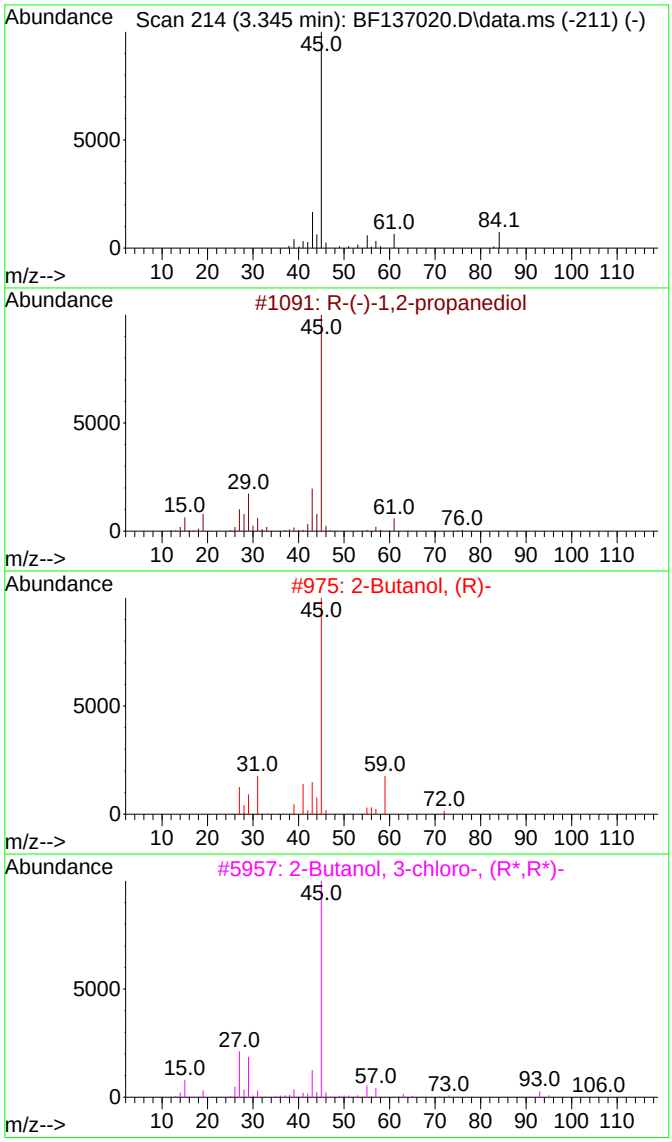
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

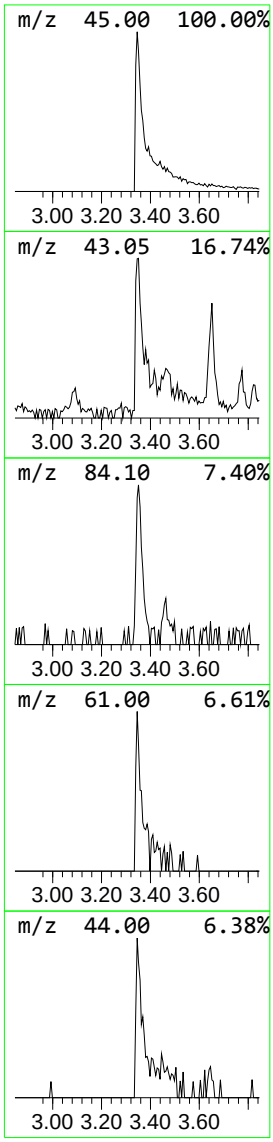
****

Peak Number 2 unknown3.345 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.345	5.55 ng	78730	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	40
3	2-Butanol, 3-chloro-, (R*,R*)-	108	C4H9ClO	010325-40-3	40
4	2-Butanol, 3-chloro-, (R*,S*)-	108	C4H9ClO	010325-41-4	40
5	2-Hexanol	102	C6H14O	000626-93-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

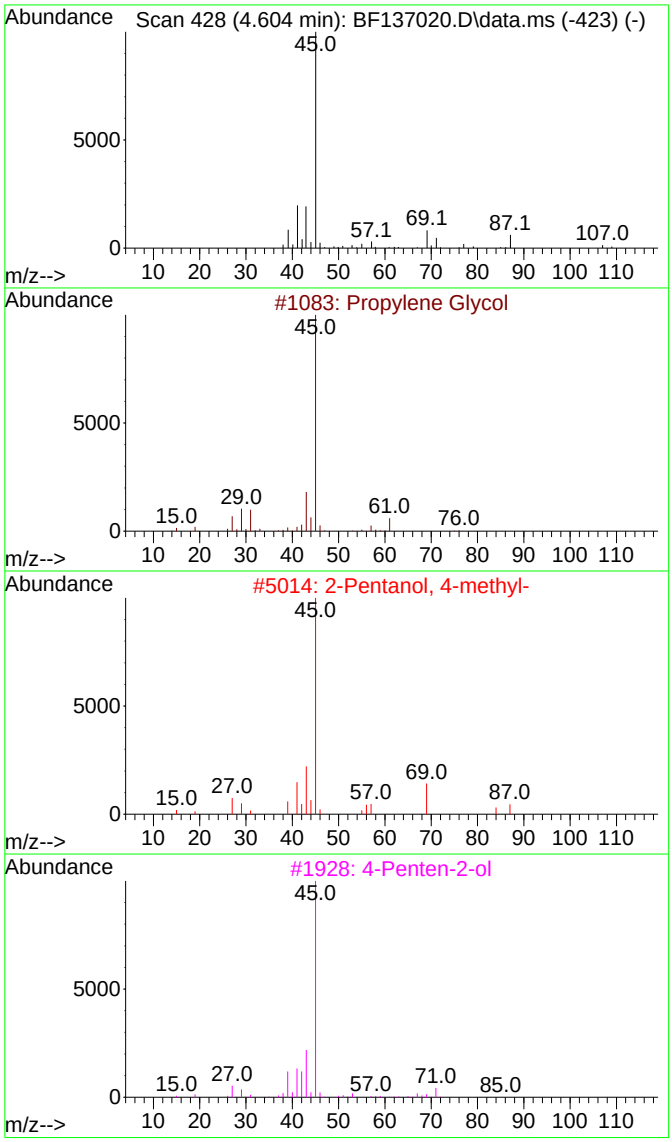
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

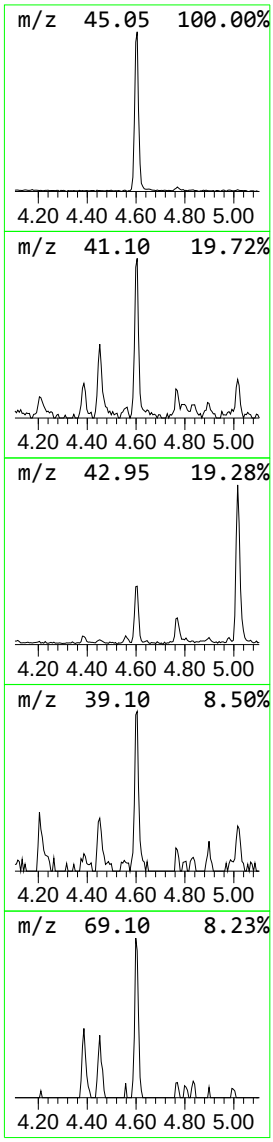
****

Peak Number 3 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.604	6.91 ng	98029	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	50
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	39
3	4-Penten-2-ol	86	C5H10O	000625-31-0	39
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	39
5	Diisopropyl ether	102	C6H14O	000108-20-3	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

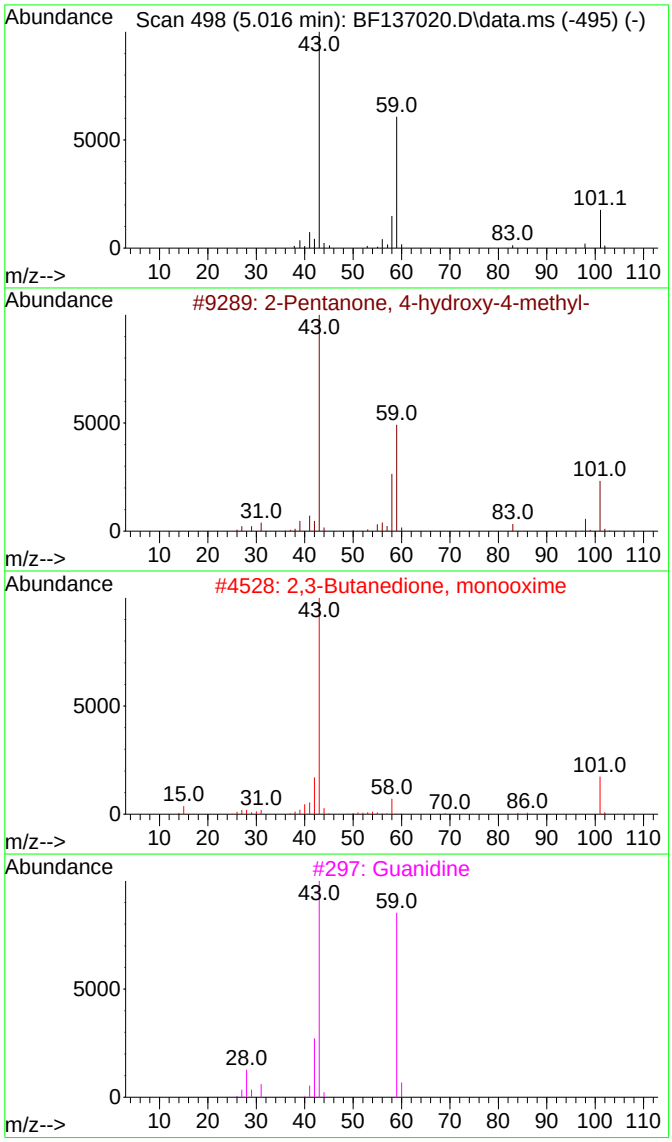
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

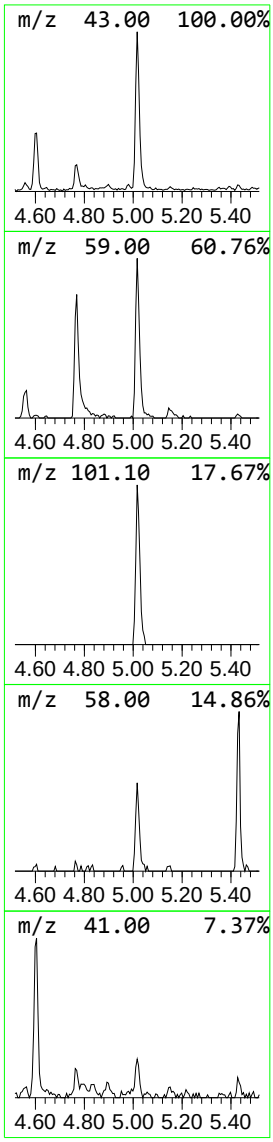
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	4.29 ng	60918	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Guanidine	59	CH5N3	000113-00-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

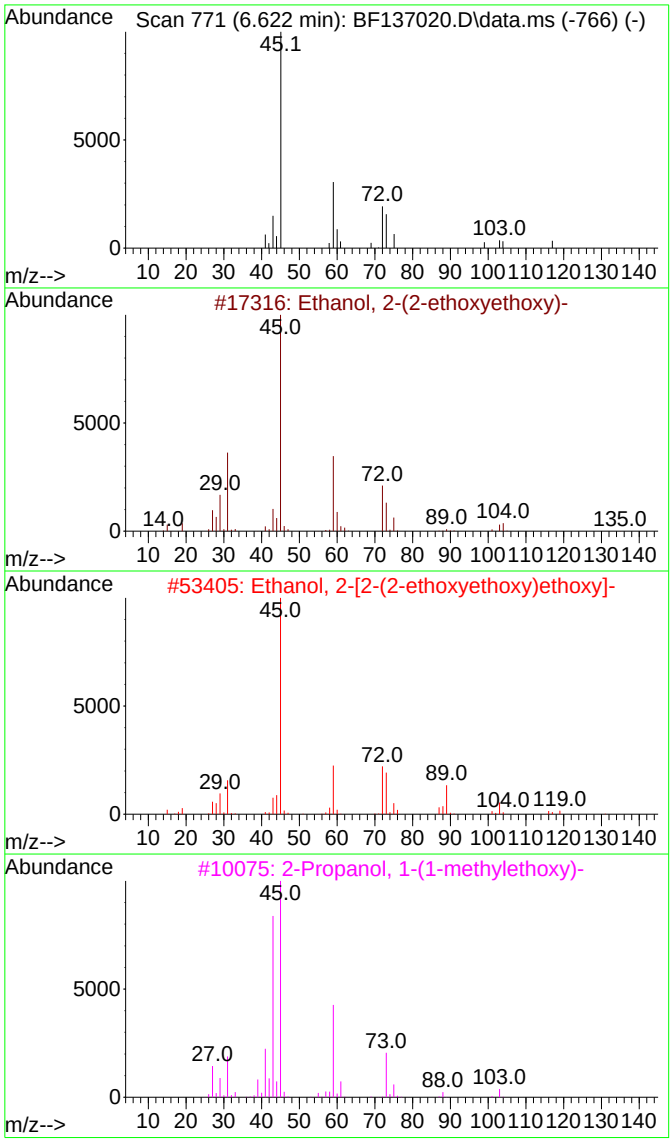
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

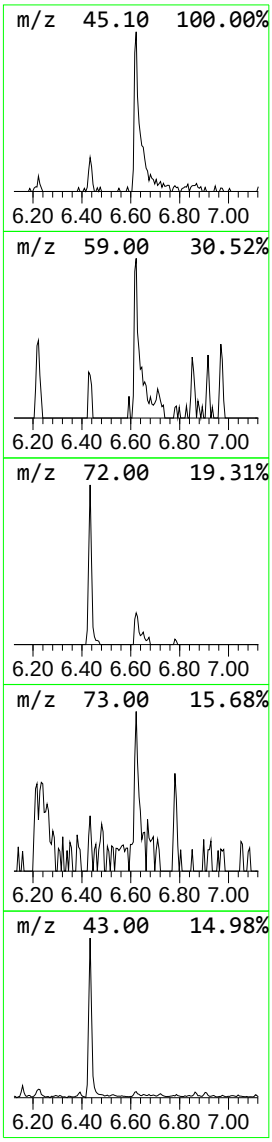
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	2.00 ng	28385	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
4	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9
5	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

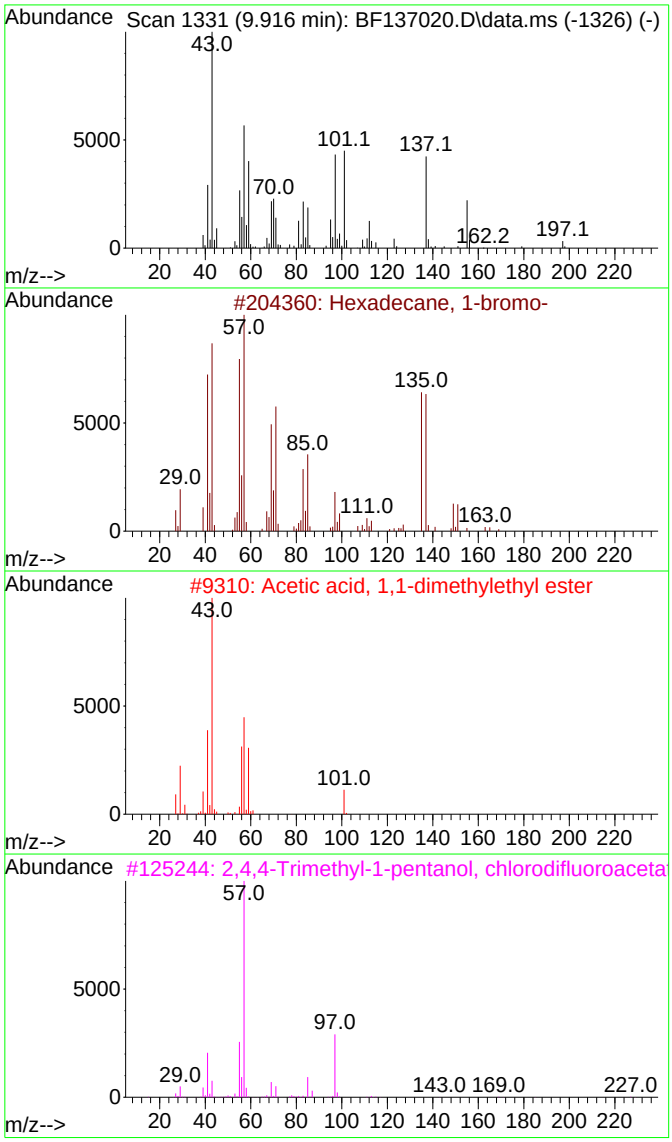
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

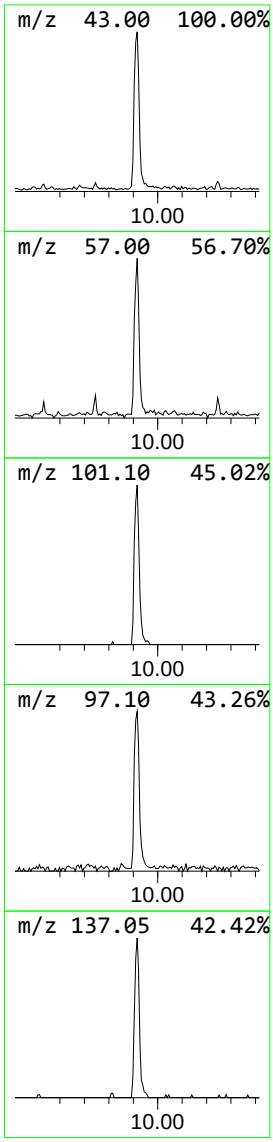
****

Peak Number 6 unknown9.916 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	12.60 ng	211988	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	22
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
3	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
4	Butyl decyl ether	214	C14H30O	1000406-40-2	10
5	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

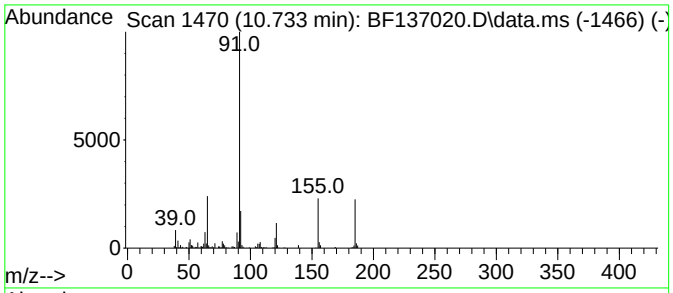
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

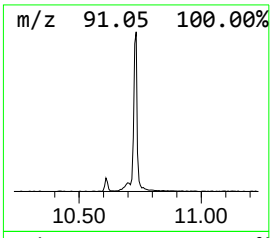
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

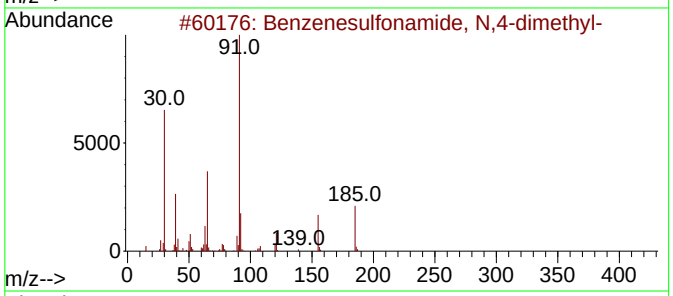
****
Peak Number 7 Benzenesulfonamide, N,4-dim... Concentration Rank 2

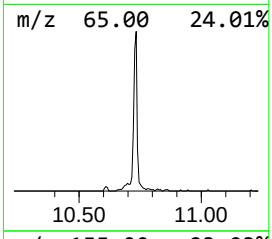
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	16.71 ng	270137	Phenanthrene-d10	11.310

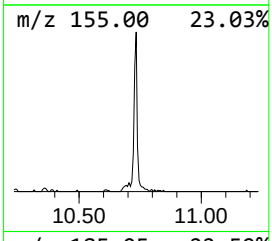
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	70
3	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
4	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47

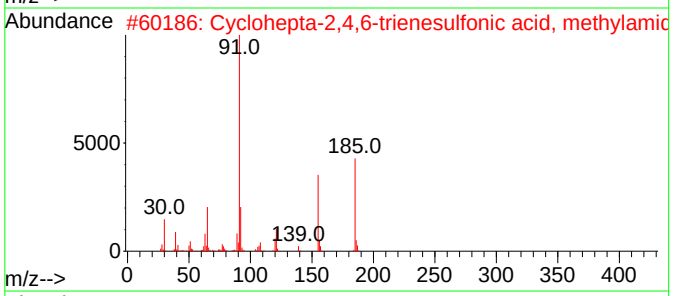


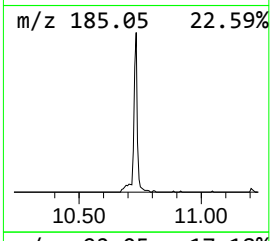


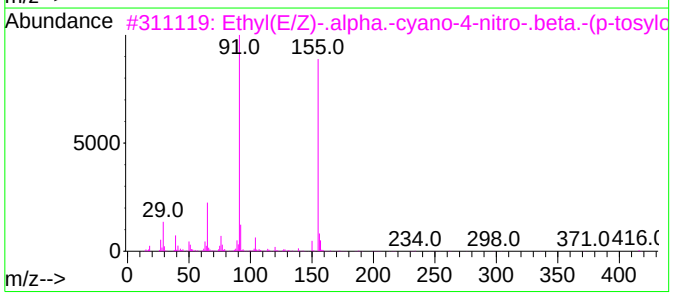


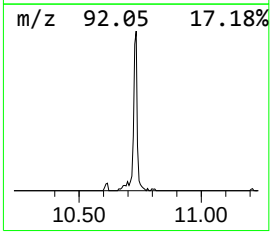












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

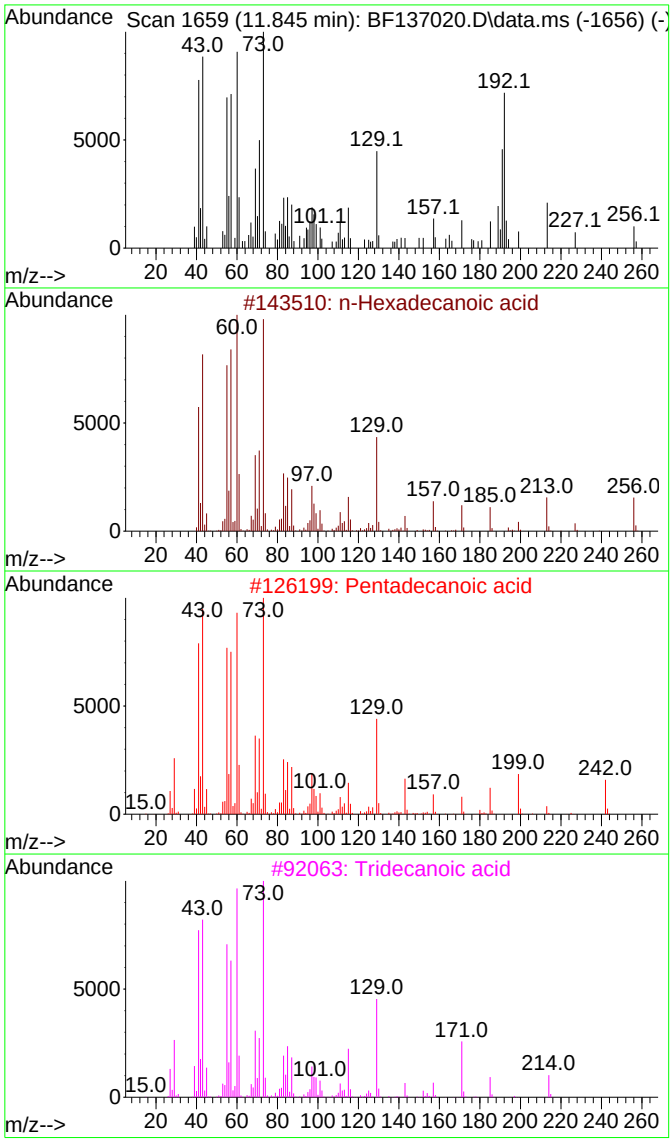
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

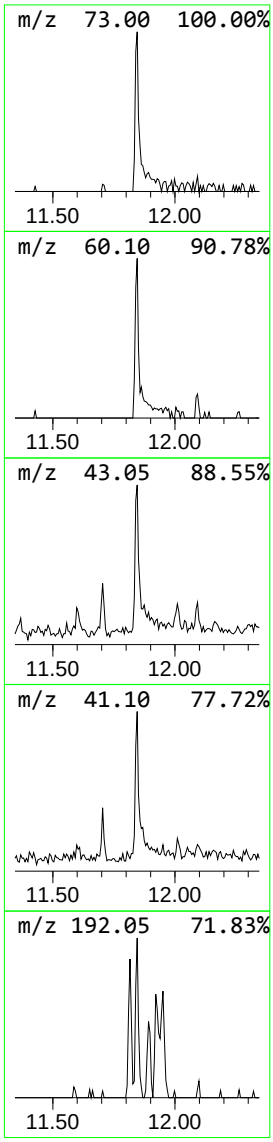
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	4.84 ng	78280	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

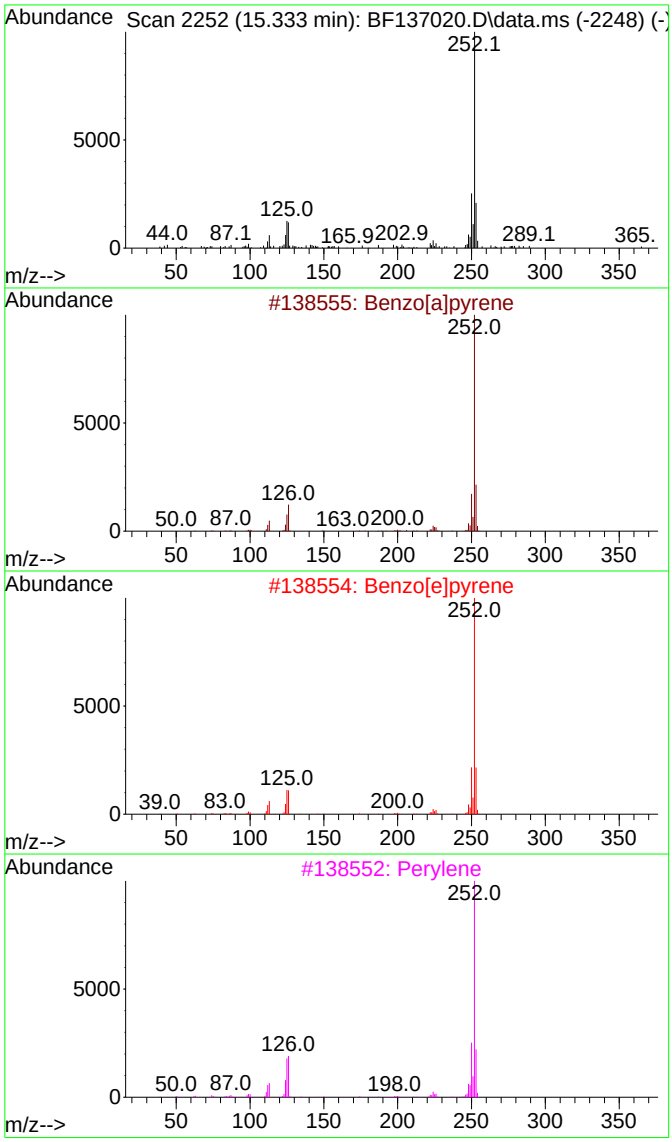
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

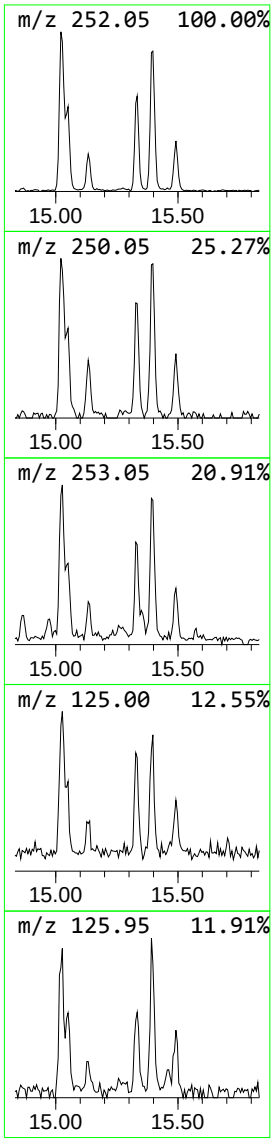
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	3.22 ng	62319	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137020.D
Acq On : 10 Jan 2024 15:15
Operator : CG\JU
Sample : P1085-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
3-Buten-2-ol, 2...	2.193	56.6	ng	803480	1	6.781	283751	20.0
unknown3.345	3.345	5.5	ng	78730	1	6.781	283751	20.0
Propylene Glycol	4.604	6.9	ng	98029	1	6.781	283751	20.0
2-Pentanone, 4-...	5.016	4.3	ng	60918	1	6.781	283751	20.0
Ethanol, 2-(2-e...	6.622	2.0	ng	28385	1	6.781	283751	20.0
unknown9.916	9.916	12.6	ng	211988	3	9.816	336543	20.0
Benzenesulfonam...	10.733	16.7	ng	270137	4	11.310	323314	20.0
n-Hexadecanoic ...	11.845	4.8	ng	78280	4	11.310	323314	20.0
Benzo[e]pyrene	15.333	3.2	ng	62319	6	15.462	387217	20.0