LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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: BF137019.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	8	18	31	rVB	530235	736594	66.74%	7.538%
2	3.346	211	214	223	rBV2	27111	58974	5.34%	0.603%
3	3.652	262	266	276	rVB4	9704	15532	1.41%	0.159%
4	3.922	308	312	320	rBV3	11076	16193	1.47%	0.166%
5	4.016	324	328	329	rBV	11359	13148	1.19%	0.135%
6	4.040	329	332	341	rVB3	12498	20545	1.86%	0.210%
7	4.210	357	361	368	rBV	8494	12843	1.16%	0.131%
8	4.387	387	391	398	rBV2	17346	22344	2.02%	0.229%
9	4.452	398	402	412	rVB	16158	22374	2.03%	0.229%
10	4.604	423	428	439	rVB	82691	95061	8.61%	0.973%
11	4.769	453	456	460	rBV	17480	21311	1.93%	0.218%
12	5.016	495	498	506	rVB	54069	62791	5.69%	0.643%
13	5.428	565	568	587	rBV	930625	937852	84.98%	9.597%
14	6.222	699	703	712	rBV4	9132	13908	1.26%	0.142%
15	6.434	735	739	754	rBV	1060286	922967	83.63%	9.445%
16	6.616	766	770	777	rBV4	12287	26806	2.43%	0.274%
17	6.781	795	798	802	rBV	366321	298647	27.06%	3.056%
18	6.863	809	812	815	rVB2	11009	12255	1.11%	0.125%
19	6.904	815	819	827	rVB2	11974	15217	1.38%	0.156%
20	7.346	890	894	897	rBV	740412	597533	54.14%	6.115%
21	7.598	935	937	945	rVB	27344	25051	2.27%	0.256%
22	8.057	1012	1015	1018	rBV	447371	360840	32.69%	3.692%
23	8.340	1059	1063	1065	rBV3	12257	15882	1.44%	0.163%
24	8.381	1065	1070	1072	rBV4	19085	26949	2.44%	0.276%
25	8.775	1134	1137	1140	rBV	18359	15418	1.40%	0.158%
26	8.869	1150	1153	1157	rBV	13874	13662	1.24%	0.140%
27	9.134	1194	1198	1202	rBV	1220071	1103677	100.00%	11.294%
28	9.475	1253	1256	1258	rBV	12070	12003	1.09%	0.123%
29	9.769	1304	1306	1309	rBV	28907	23544	2.13%	0.241%
30	9.816	1309	1314	1318	rBV	486649	386952	35.06%	3.960%
31	9.916	1325	1331	1337	rVB4	17990	30473	2.76%	0.312%
32	10.022	1345	1349	1353	rVB	20646	20711	1.88%	0.212%
33	10.363	1403	1407	1412	rBV2	10723	14533	1.32%	0.149%
34	10.610	1446	1449	1459	rBV	605946	591260	53.57%	6.050%
35	10.728	1465	1469	1477	rVB	183090	179966	16.31%	1.842%
36	11.122	1533	1536	1539	rBV	13268	11614	1.05%	0.119%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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	11.204	1547	1550	1555	rVB4	9433	11986	1.09%	0.123%
38	11.310	1565	1568	1571	rBV	442378	370180	33.54%	3.788%
39	11.333	1571	1572	1575	rVV	71969	46634	4.23%	0.477%
40	11.386	1578	1581	1585	rVB	13885	15863	1.44%	0.162%
41	11.704	1632	1635	1638	rBV	13643	12081	1.09%	0.124%
42	11.816	1651	1654	1656	rBV2	11180	12098	1.10%	0.124%
43	11.845	1656	1659	1665	rVV	107571	108978	9.87%	1.115%
44	12.369	1745	1748	1750	rBV2	14850	13945	1.26%	0.143%
45	12.404	1751	1754	1757	rBV	15769	13847	1.25%	0.142%
46	12.533	1773	1776	1779	rBV	100723	87174	7.90%	0.892%
47	12.633	1790	1793	1797	rBV5	23217	29444	2.67%	0.301%
48	12.763	1809	1815	1820	rVV	82311	95420	8.65%	0.976%
49	12.822	1821	1825	1828	rVB5	11953	15548	1.41%	0.159%
50	12.904	1835	1839	1843	rBV	924758	819803	74.28%	8.389%
51	13.075	1864	1868	1869	rBV4	11895	13875	1.26%	0.142%
52	13.198	1887	1889	1897	rVB6	13707	17328	1.57%	0.177%
53	13.322	1908	1910	1915	rBV6	8013	13802	1.25%	0.141%
54	13.480	1933	1937	1940	rBV6	14962	19428	1.76%	0.199%
55	13.610	1957	1959	1961	rBV	13149	11681	1.06%	0.120%
56	13.722	1975	1978	1980	rBV3	13680	12325	1.12%	0.126%
57	13.886	2001	2006	2009	rBV5	24093	48504	4.39%	0.496%
58	13.969	2013	2020	2023	rVV2	348071	381487	34.57%	3.904%
59	13.998	2023	2025	2032	rVB	52688	57023	5.17%	0.584%
60	14.063	2034	2036	2040	rVB4	10791	13581	1.23%	0.139%
61	14.127	2045	2047	2050	rBV4	11829	12580	1.14%	0.129%
62	14.322	2078	2080	2083	rBV4	9544	12783	1.16%	0.131%
63	14.363	2085	2087	2090	rVB2	16443	13524	1.23%	0.138%
64	14.392	2090	2092	2096	rBV3	13029	12029	1.09%	0.123%
65	14.439	2097	2100	2105	rVB6	18119	22787	2.06%	0.233%
66	14.486	2105	2108	2110	rBV3	10241	13022	1.18%	0.133%
67	14.863	2169	2172	2174	rBV3	12968	15237	1.38%	0.156%
68	15.021	2196	2199	2202	rBV	63278	86339	7.82%	0.884%
69	15.333	2248	2252	2258	rVB	39102	53739	4.87%	0.550%
70	15.398	2259	2263	2268	rVB	44566	54695	4.96%	0.560%
71	15.463	2269	2274	2284	rBV	281701	380449	34.47%	3.893%
72	15.927	2349	2353	2355	rBV5	9969	12994	1.18%	0.133%
73	16.592	2464	2466	2472	rBV7	8048	13250	1.20%	0.136%
74	16.980	2528	2532	2541	rVB3	22832	47584	4.31%	0.487%
75	17.439	2608	2610	2616	rVB3	13398	23800	2.16%	0.244%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

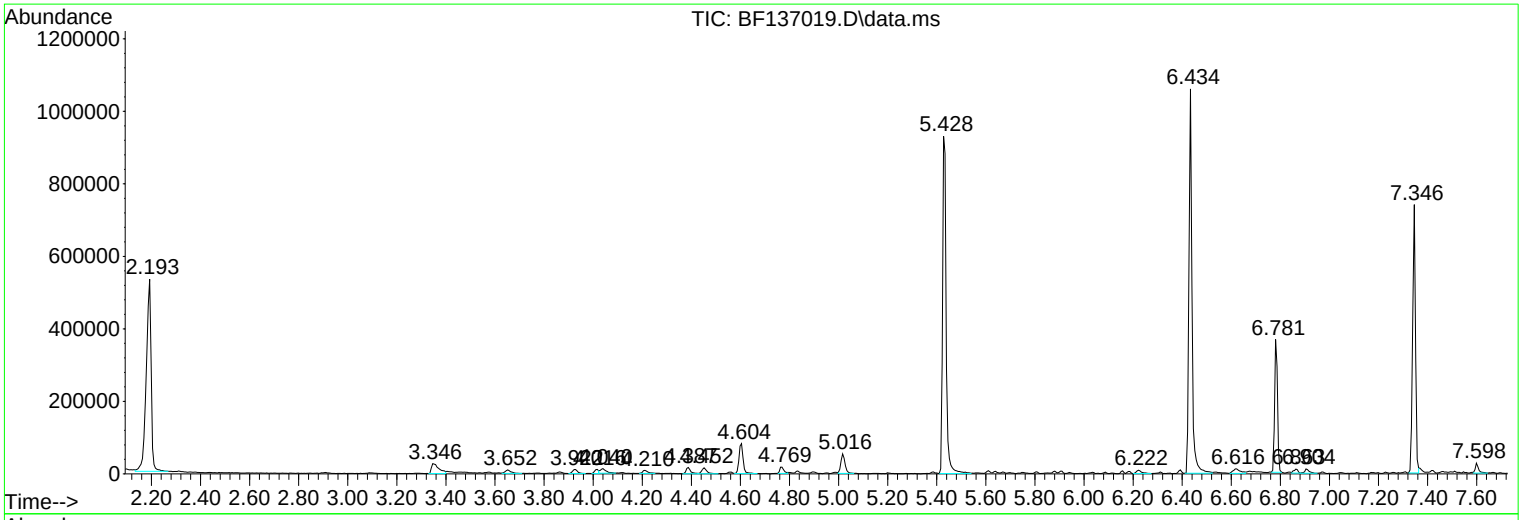
Sum of corrected areas: 9772277

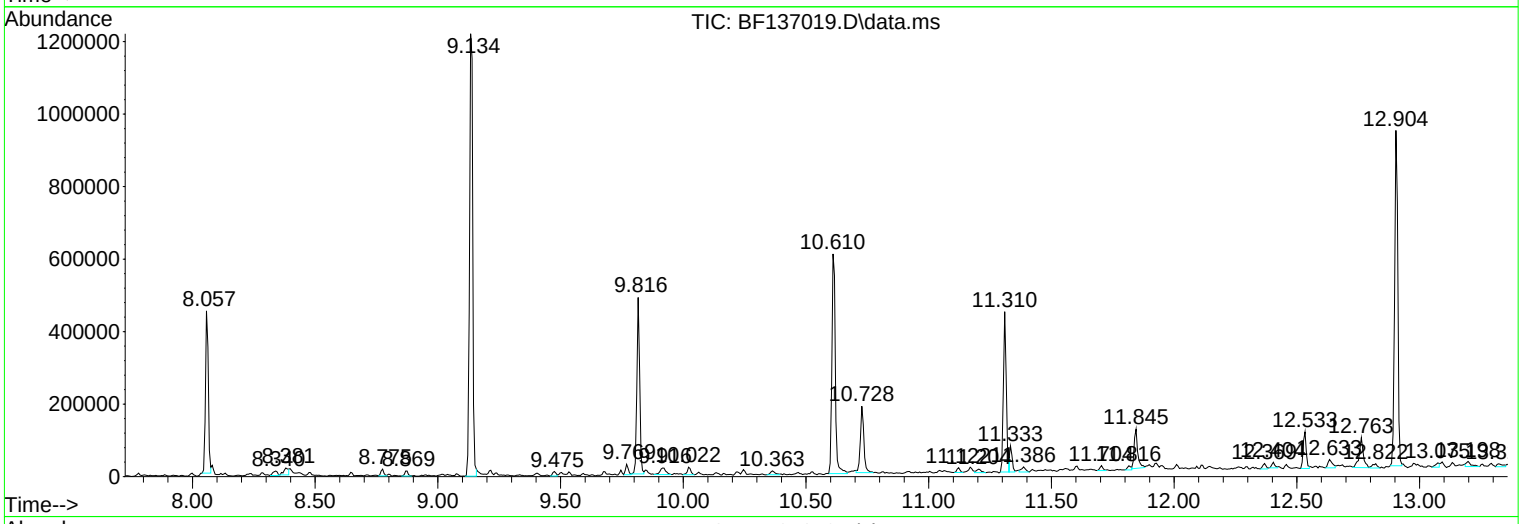
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

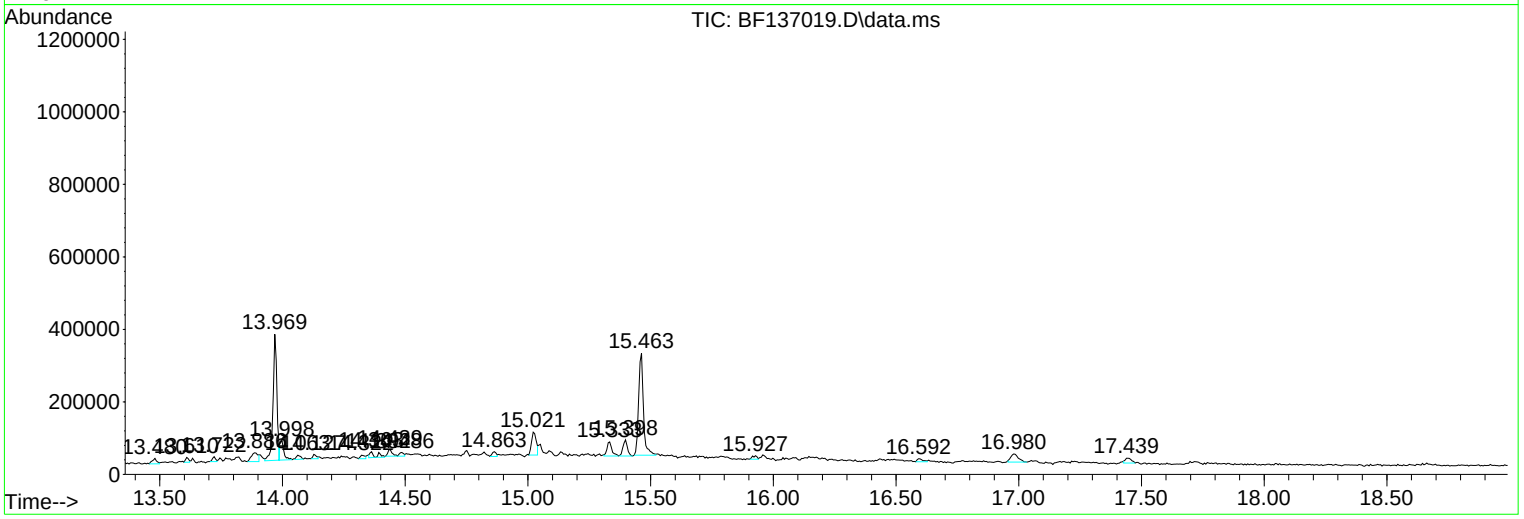
Instrument :
BNA_F
ClientSampleId :
TP-2

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 : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

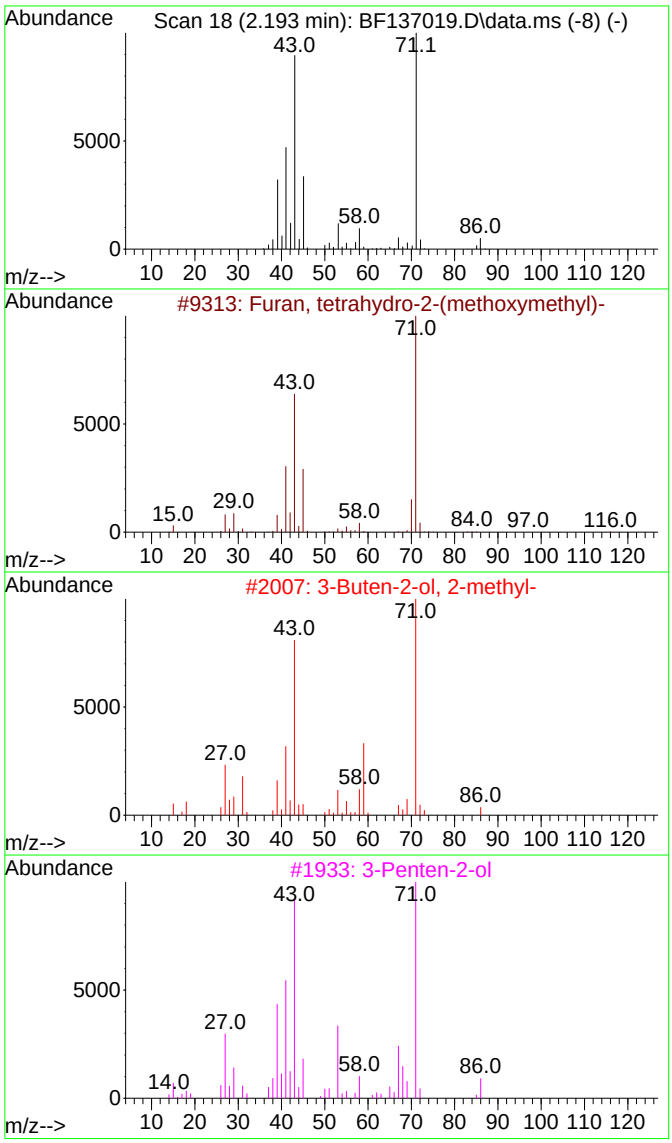
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

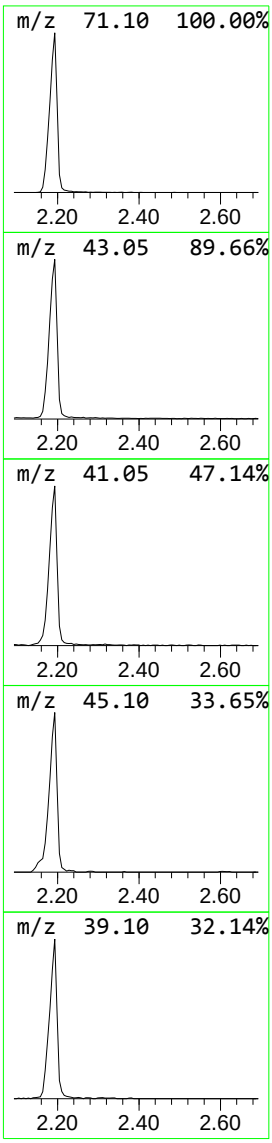
****

Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	49.33 ng	736594	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
3	3-Penten-2-ol	86	C5H10O	001569-50-2	64
4	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	59
5	Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

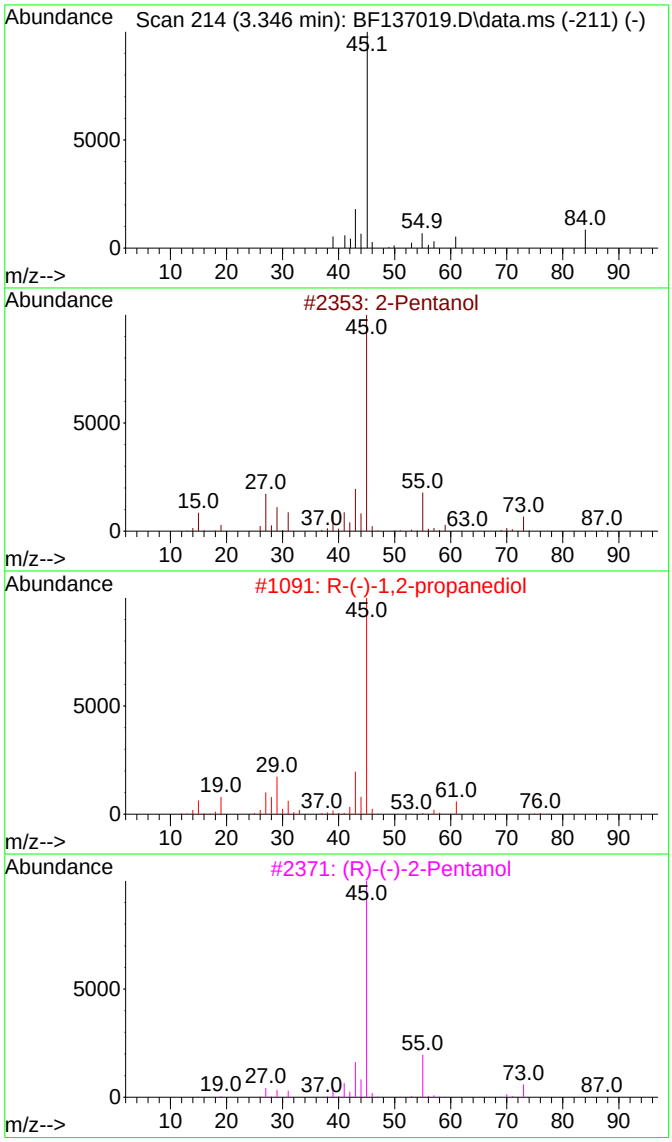
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

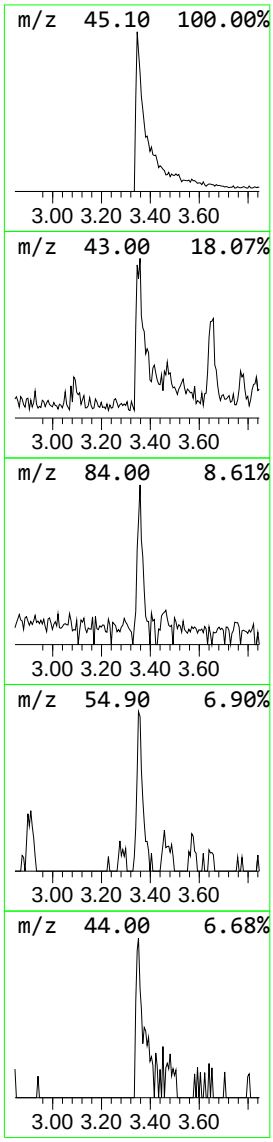
****

Peak Number 2 unknown3.346 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	3.95 ng	58974	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol	88	C5H12O	006032-29-7	40
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	39
4	2-Hexanol	102	C6H14O	000626-93-7	9
5	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

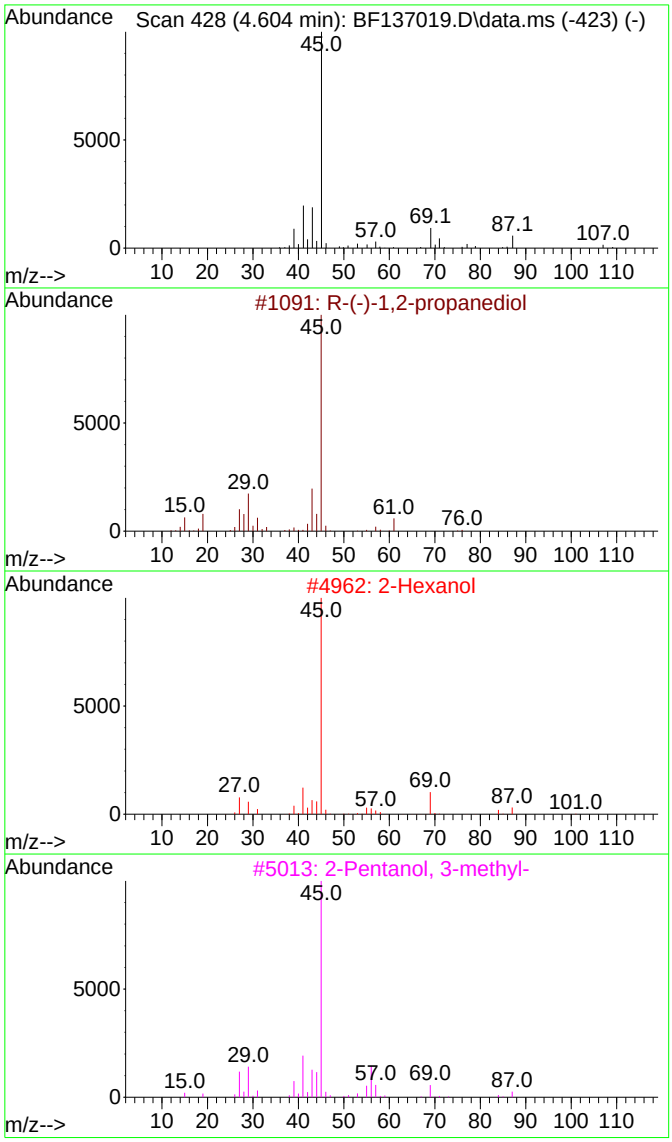
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

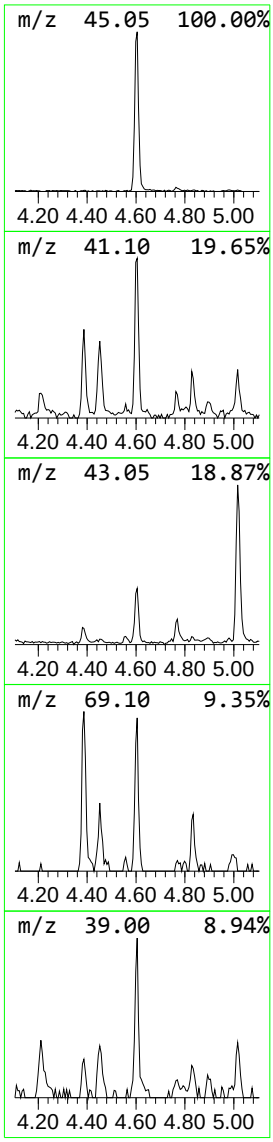
****

Peak Number 3 unknown4.604 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.604	6.37 ng	95061	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	45
2	2-Hexanol	102	C6H14O	000626-93-7	40
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	40
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	38
5	4-Penten-2-ol	86	C5H10O	000625-31-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
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ALS Vial : 10 Sample Multiplier: 1

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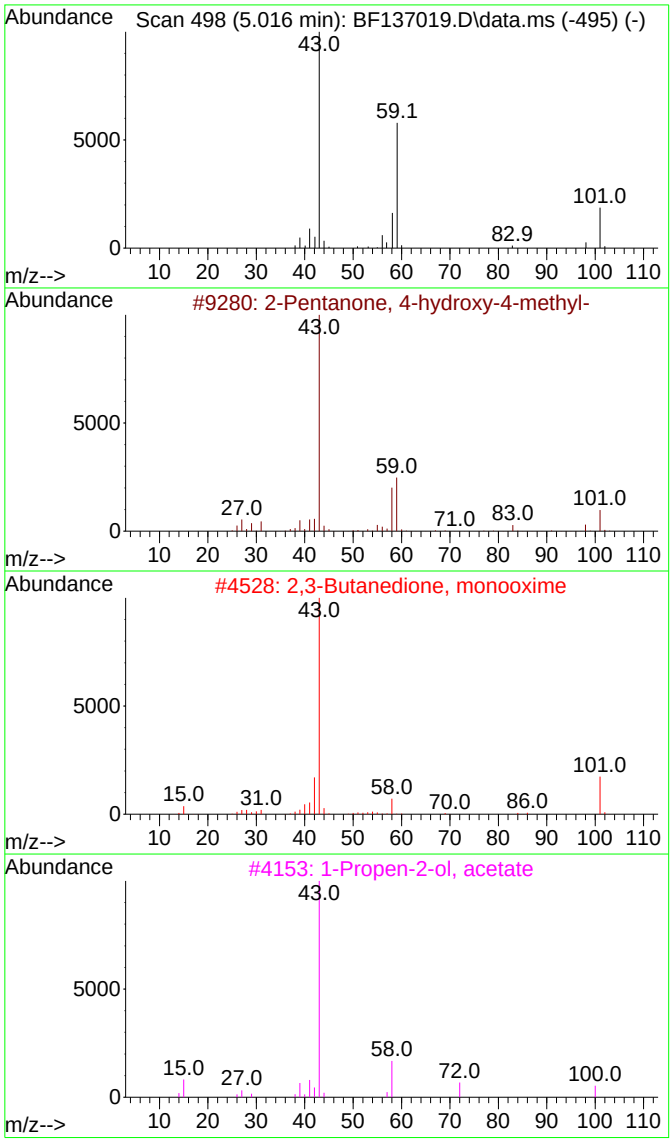
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

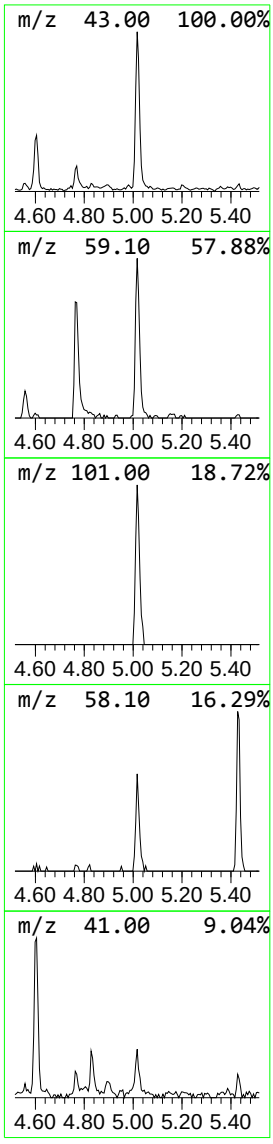
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	4.21 ng	62791	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	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16
4	Acetone	58	C3H6O	000067-64-1	16
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

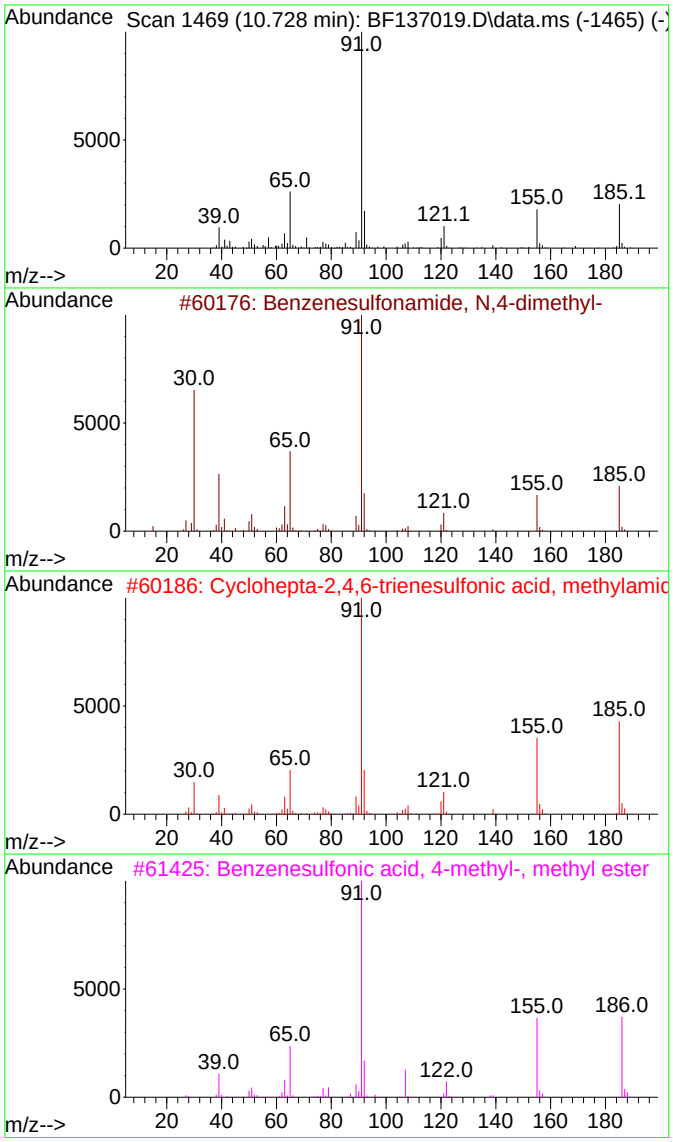
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

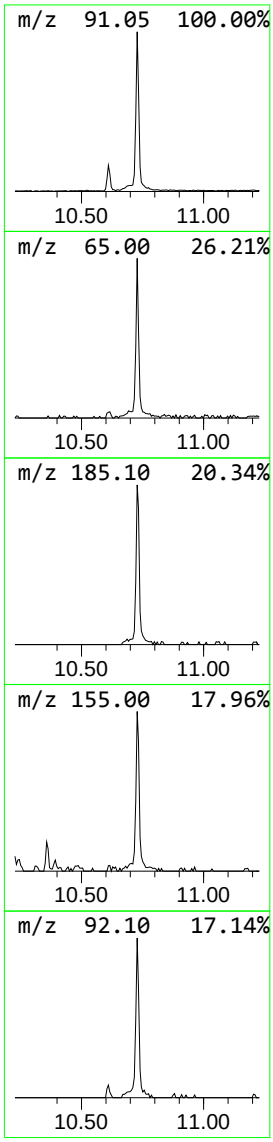
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.728	9.72 ng	179966	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	76
3	Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	50
4	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	47
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

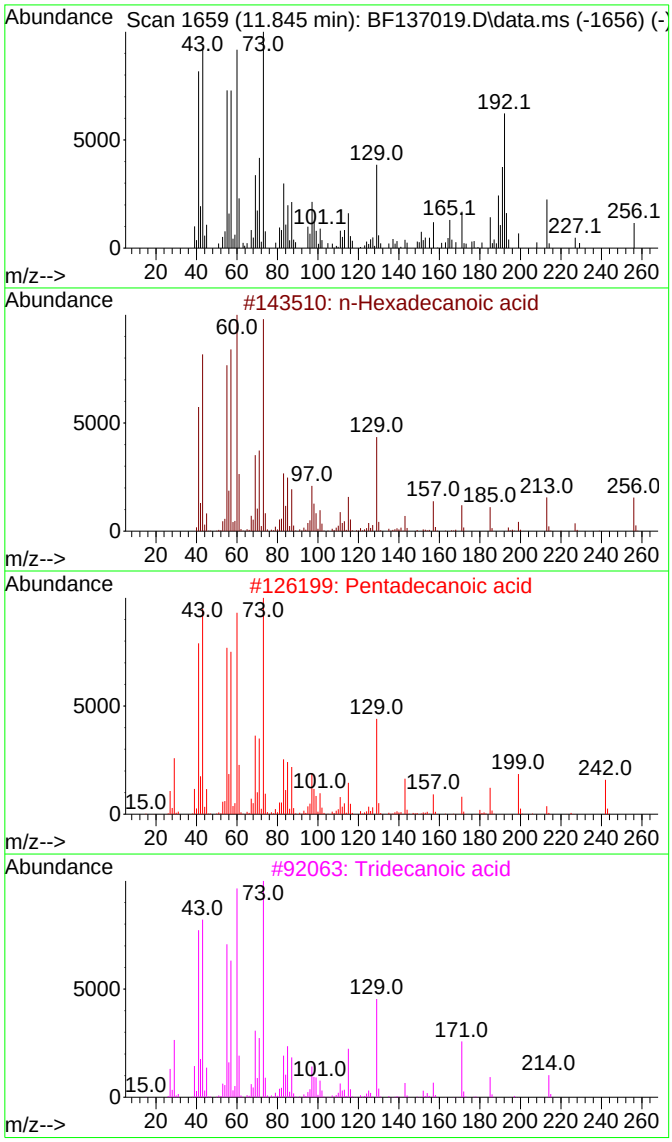
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

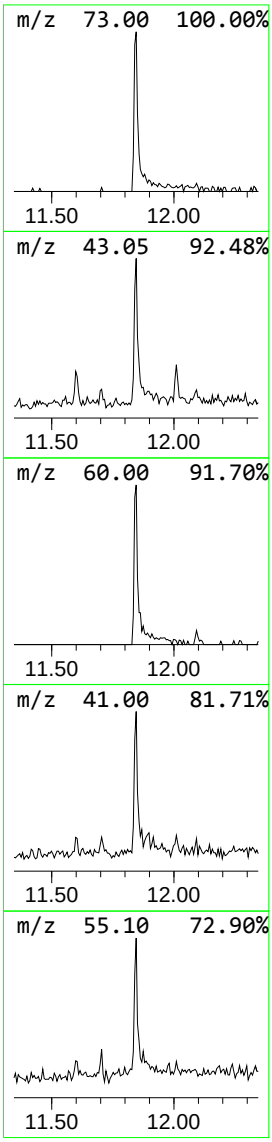
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	5.89 ng	108978	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	49





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Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

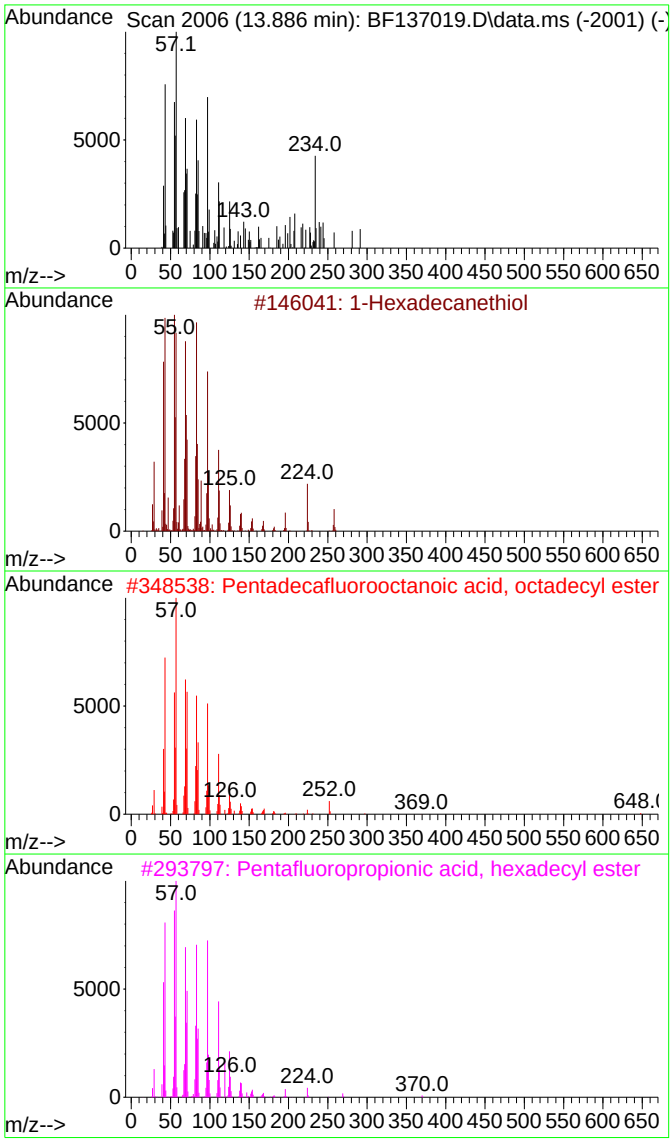
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

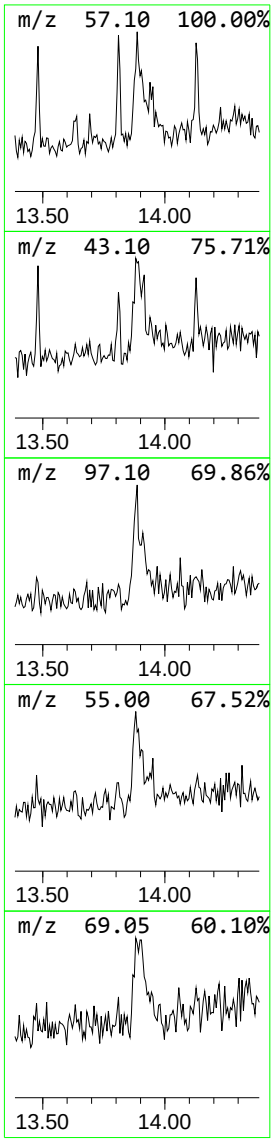
****

Peak Number 7 unknown13.886 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.54 ng	48504	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	49
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	43
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	38
4	Cyclododecane, ethyl-	196	C14H28	028981-49-9	38
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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

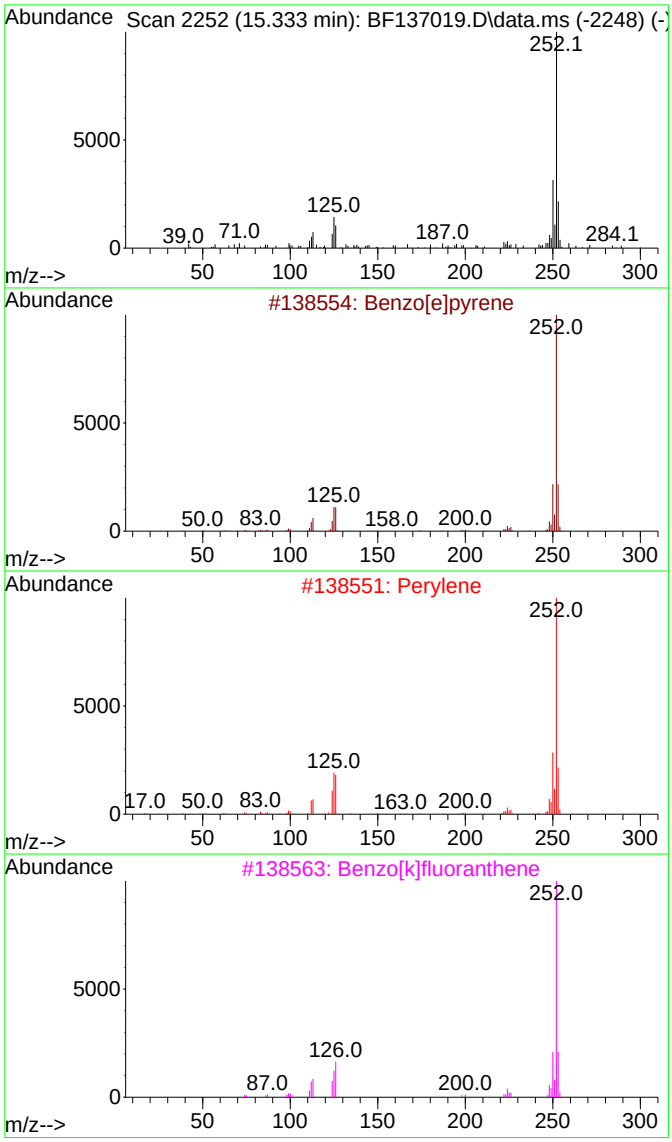
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

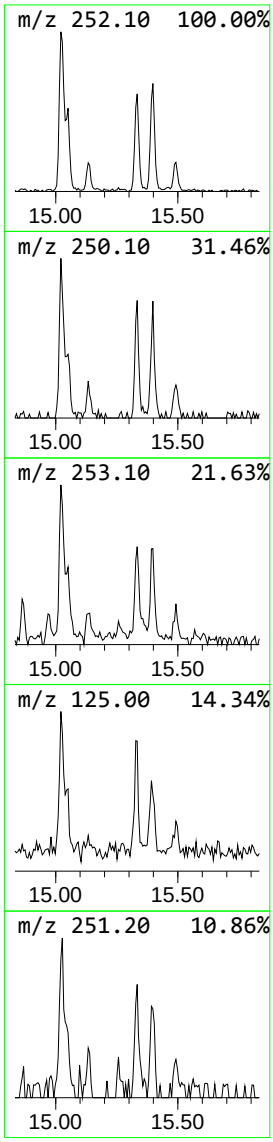
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	2.83 ng	53739	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137019.D
Acq On : 10 Jan 2024 14:43
Operator : CG\JU
Sample : P1085-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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
Furan, tetrahyd...	2.193	49.3	ng	736594	1	6.781	298647	20.0
unknown3.346	3.346	4.0	ng	58974	1	6.781	298647	20.0
unknown4.604	4.604	6.4	ng	95061	1	6.781	298647	20.0
2-Pentanone, 4-...	5.016	4.2	ng	62791	1	6.781	298647	20.0
Benzenesulfonam...	10.728	9.7	ng	179966	4	11.310	370180	20.0
n-Hexadecanoic ...	11.845	5.9	ng	108978	4	11.310	370180	20.0
unknown13.886	13.886	2.5	ng	48504	5	13.969	381487	20.0
Benzo[e]pyrene	15.333	2.8	ng	53739	6	15.463	380449	20.0