LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BIN-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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	11	19	26	rVB	816041	1257056	72.32%	8.720%
2	5.099	503	511	520	rBB	69711	104687	6.02%	0.726%
3	5.499	572	579	584	rBV	1091519	1468470	84.49%	10.187%
4	6.498	743	749	755	rBV	1070763	1534764	88.30%	10.646%
5	6.875	808	813	818	rBB	322404	384352	22.11%	2.666%
6	7.440	902	909	914	rBV	728973	985698	56.71%	6.838%
7	7.687	947	951	956	rVB	24022	29249	1.68%	0.203%
8	8.157	1025	1031	1036	rBV	397620	484412	27.87%	3.360%
9	9.234	1208	1214	1219	rBV	1364073	1738142	100.00%	12.057%
10	9.910	1323	1329	1333	rBV	419909	520607	29.95%	3.611%
11	10.622	1445	1450	1457	rVB	114498	140315	8.07%	0.973%
12	10.692	1457	1462	1475	rBV	764104	1000000	57.53%	6.937%
13	11.392	1576	1581	1590	rBV2	385905	637199	36.66%	4.420%
14	11.463	1590	1593	1597	rBV	19199	23062	1.33%	0.160%
15	11.622	1614	1620	1628	rBV	9969	18844	1.08%	0.131%
16	11.922	1661	1671	1681	rBV	217185	354755	20.41%	2.461%
17	12.004	1681	1685	1693	rVB2	31270	59107	3.40%	0.410%
18	12.210	1717	1720	1724	rVB	16881	21746	1.25%	0.151%
19	12.522	1771	1773	1780	rVB2	11832	17624	1.01%	0.122%
20	12.604	1781	1787	1799	rBV	214185	303035	17.43%	2.102%
21	12.698	1799	1803	1810	rBV2	24217	37093	2.13%	0.257%
22	12.828	1818	1825	1831	rBV	166417	257865	14.84%	1.789%
23	12.975	1842	1850	1855	rBV	918392	1177703	67.76%	8.170%
24	13.045	1857	1862	1870	rBV3	17062	34680	2.00%	0.241%
25	13.157	1873	1881	1885	rVB2	26411	48410	2.79%	0.336%
26	13.222	1886	1892	1895	rBV2	19131	32339	1.86%	0.224%
27	13.257	1895	1898	1902	rVB2	14602	18694	1.08%	0.130%
28	13.551	1942	1948	1957	rBV9	9943	28963	1.67%	0.201%
29	13.663	1961	1967	1975	rVV	19859	33650	1.94%	0.233%
30	13.774	1981	1986	1989	rBV2	18881	33067	1.90%	0.229%
31	13.874	1999	2003	2021	rVB4	49570	119078	6.85%	0.826%
32	14.027	2021	2029	2041	rVB2	286976	571398	32.87%	3.964%
33	14.410	2090	2094	2097	rBV	16100	18879	1.09%	0.131%
34	14.510	2105	2111	2112	rBV5	15766	28803	1.66%	0.200%
35	14.657	2132	2136	2140	rBV3	18736	24071	1.38%	0.167%
36	14.880	2170	2174	2181	rVB	55330	80011	4.60%	0.555%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.063	2200	2205	2214	rVB	82280	183633	10.56%	1.274%
38	15.145	2215	2219	2222	rBV	17788	26453	1.52%	0.184%
39	15.369	2252	2257	2262	rVB	42339	66839	3.85%	0.464%
40	15.427	2262	2267	2273	rVV	51879	80174	4.61%	0.556%
41	15.492	2273	2278	2291	rVB	167025	289498	16.66%	2.008%
42	15.968	2354	2359	2365	rVB	11452	19775	1.14%	0.137%
43	16.204	2395	2399	2409	rVB	6674	18906	1.09%	0.131%
44	16.768	2489	2495	2505	rVB8	11456	28191	1.62%	0.196%
45	16.951	2520	2526	2535	rVB2	18591	40703	2.34%	0.282%
46	17.392	2596	2601	2611	rVB	14312	33764	1.94%	0.234%

Sum of corrected areas: 14415764

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
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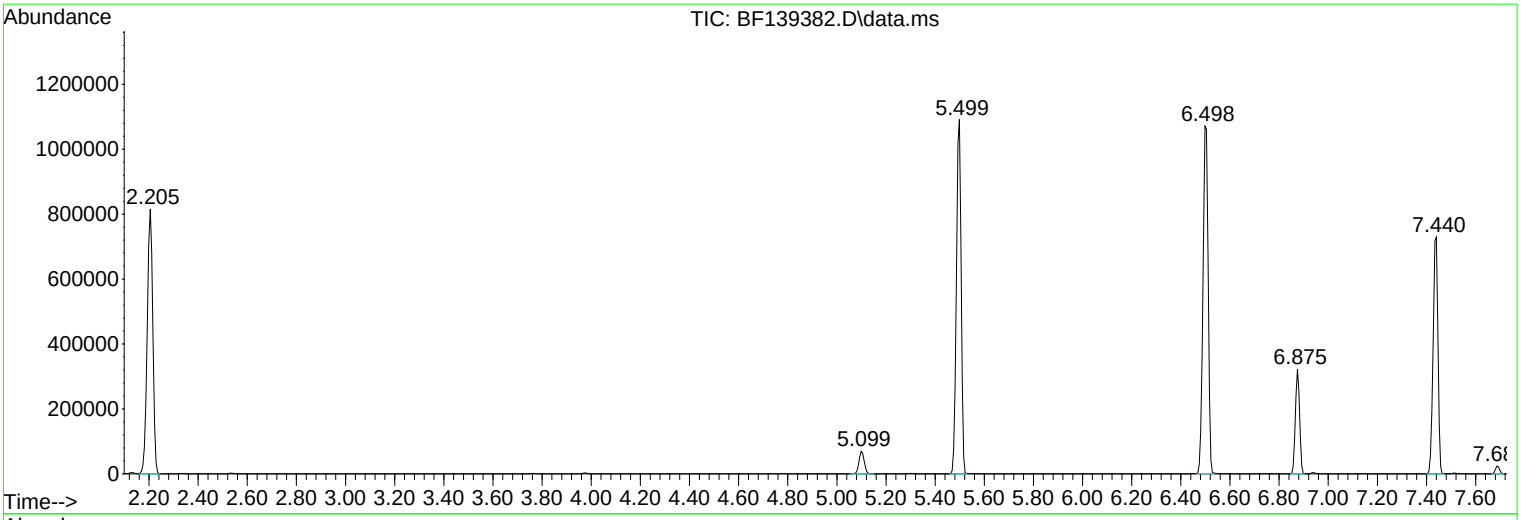
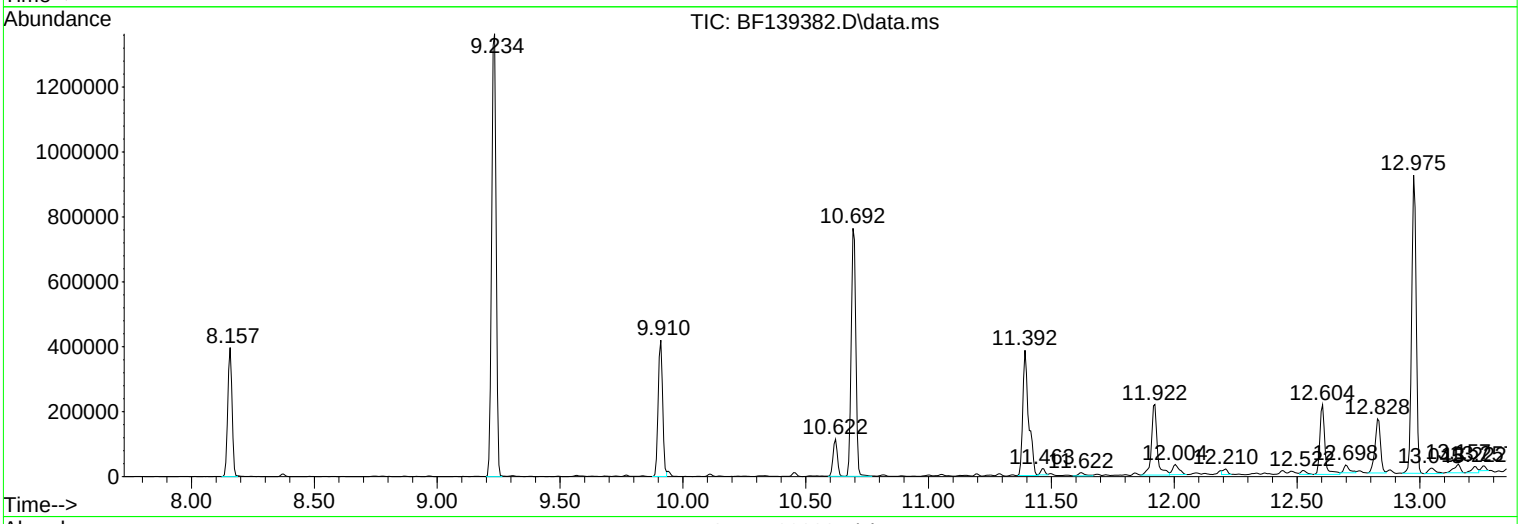
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

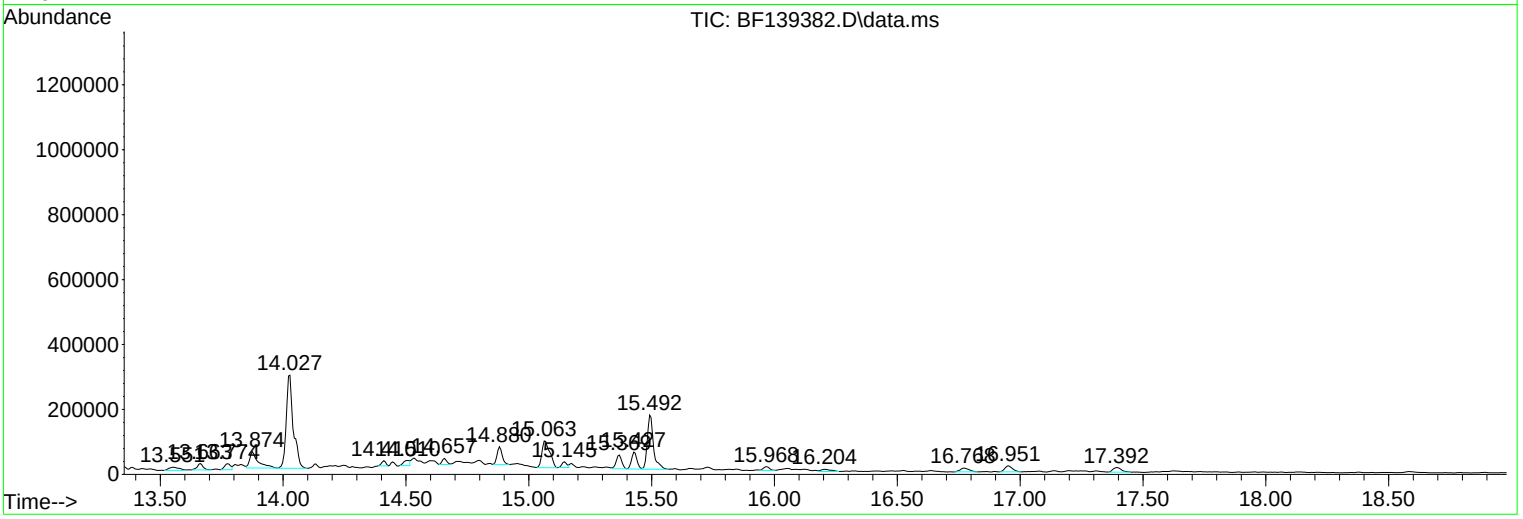
Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

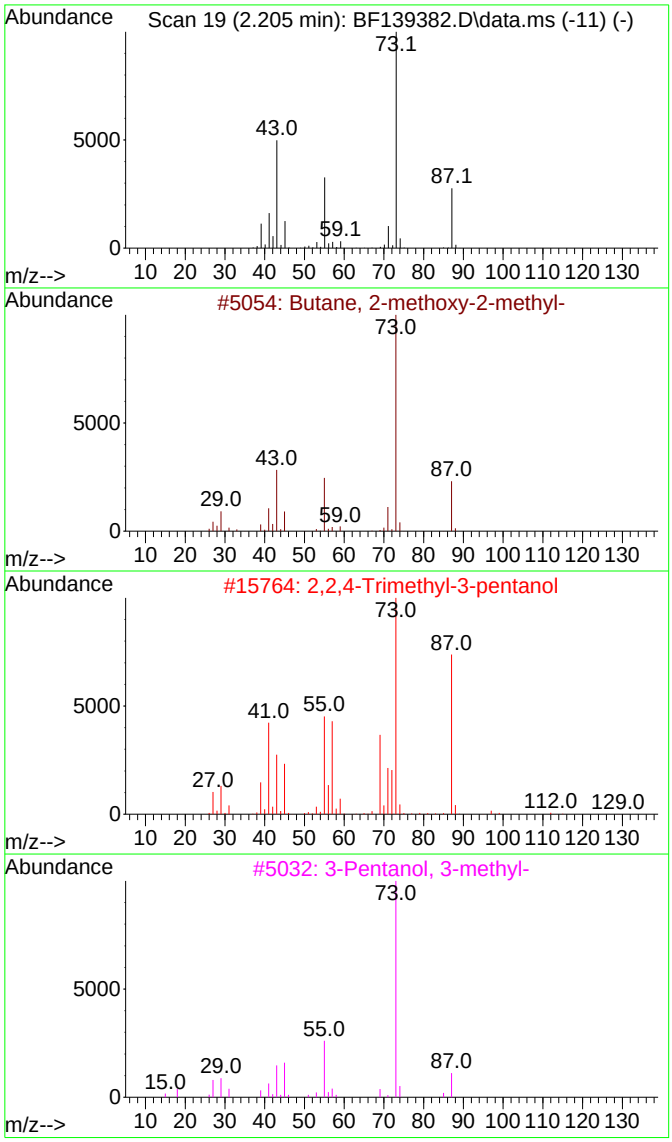
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

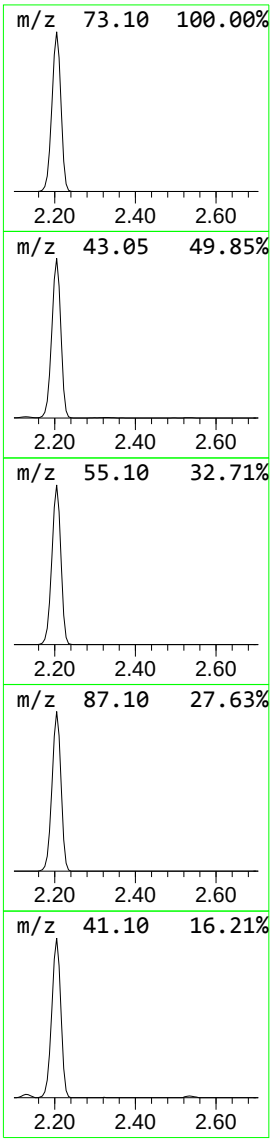
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	65.41 ng	1257060	1,4-Dichlorobenzene-d4	6.875

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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

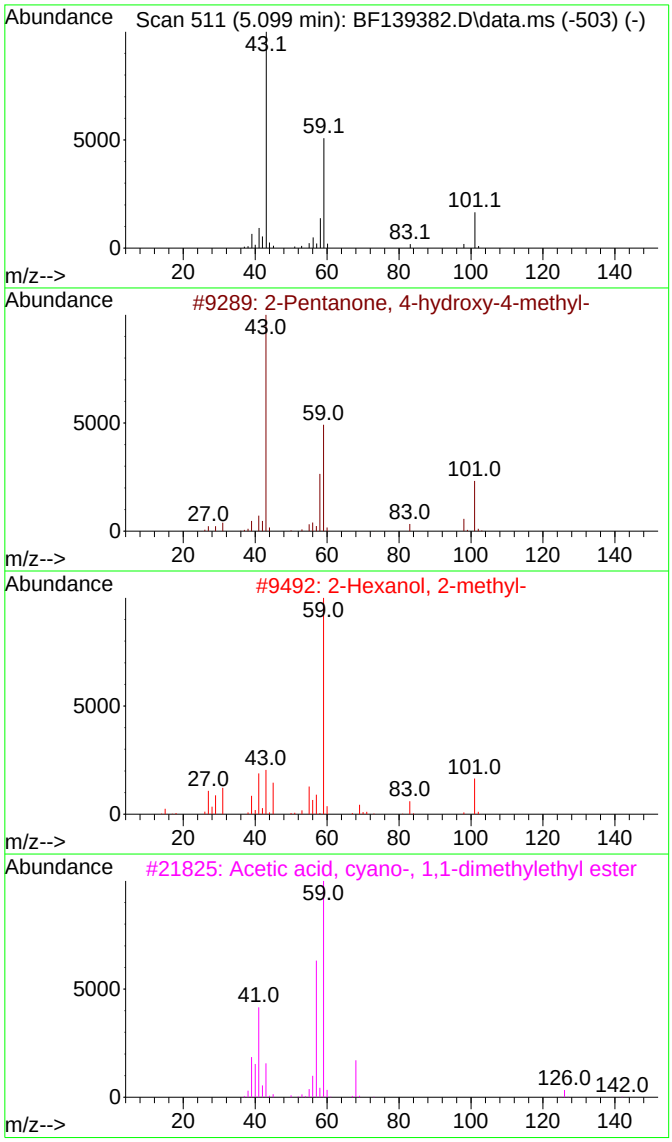
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

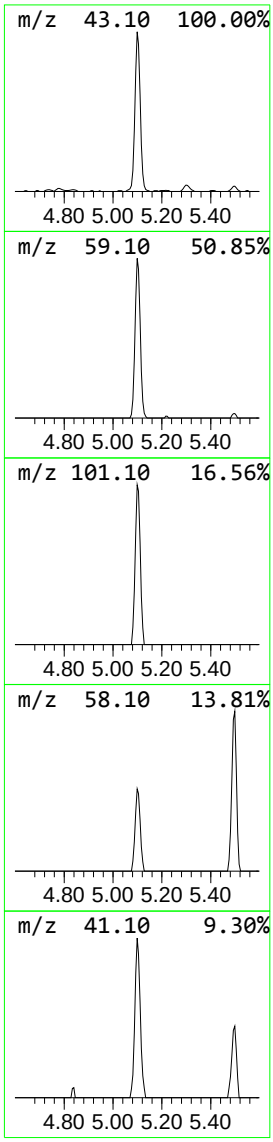
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	5.45 ng	104687	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

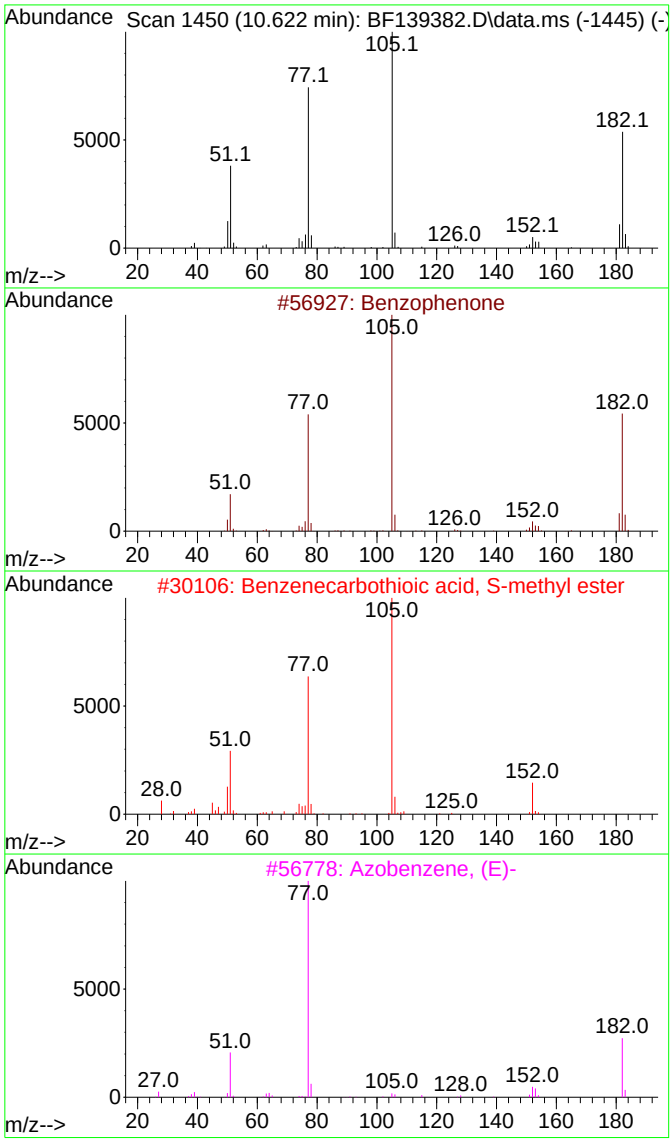
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

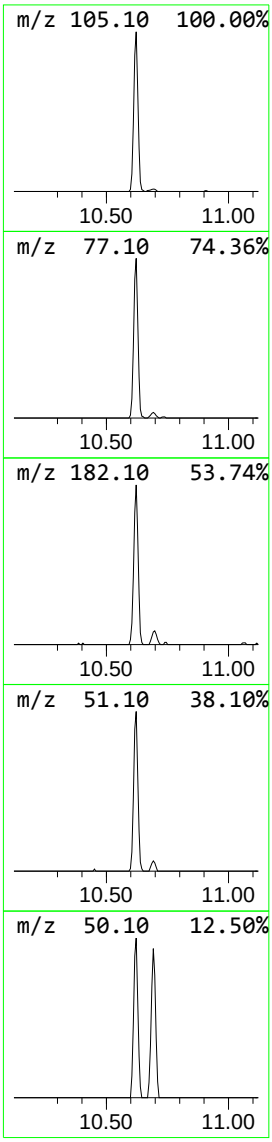
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.39 ng	140315	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	58
5	Benzoylformic acid	150	C8H6O3	000611-73-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

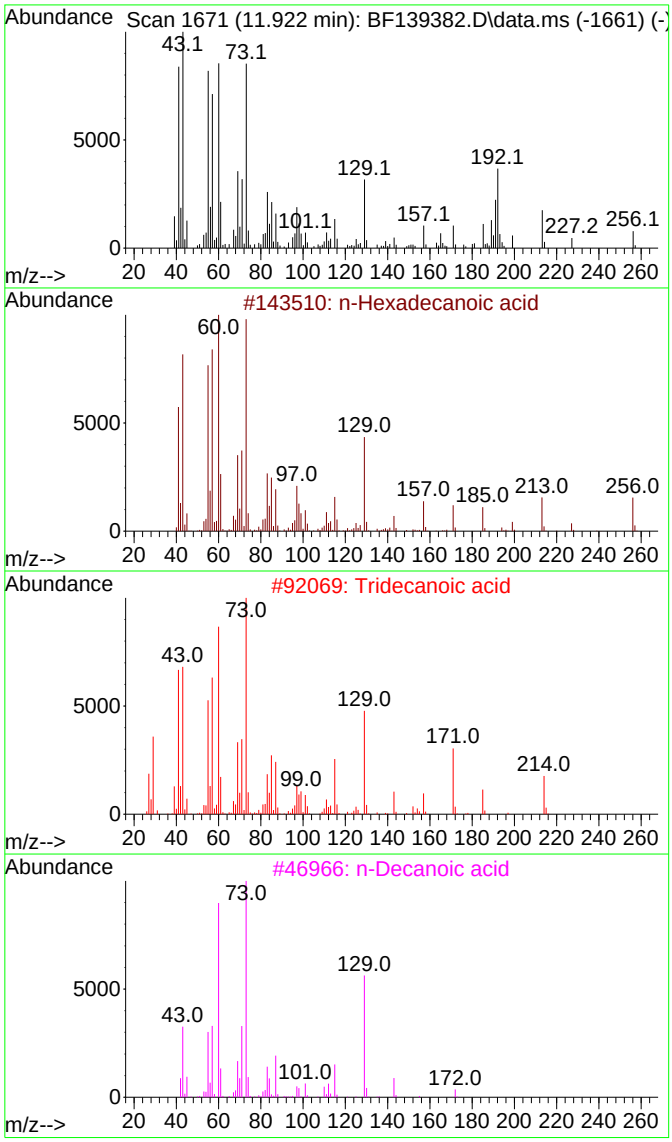
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

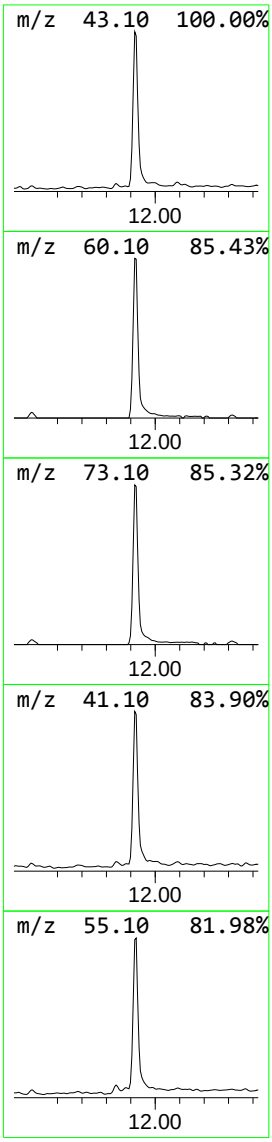
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	11.13 ng	354755	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

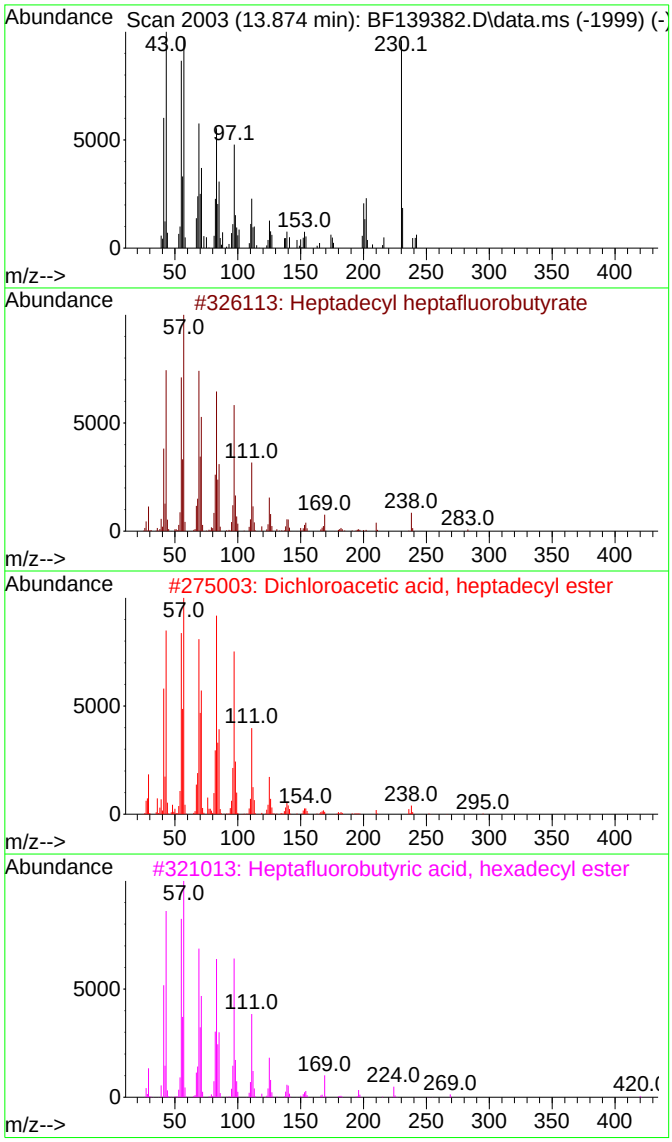
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

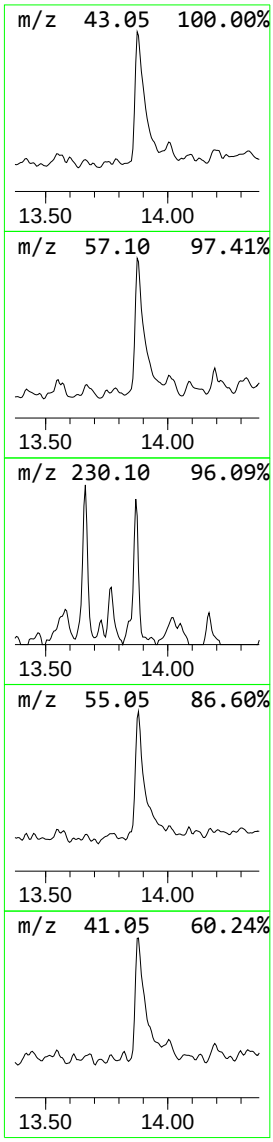
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.17 ng	119078	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	50
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	50
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	46
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

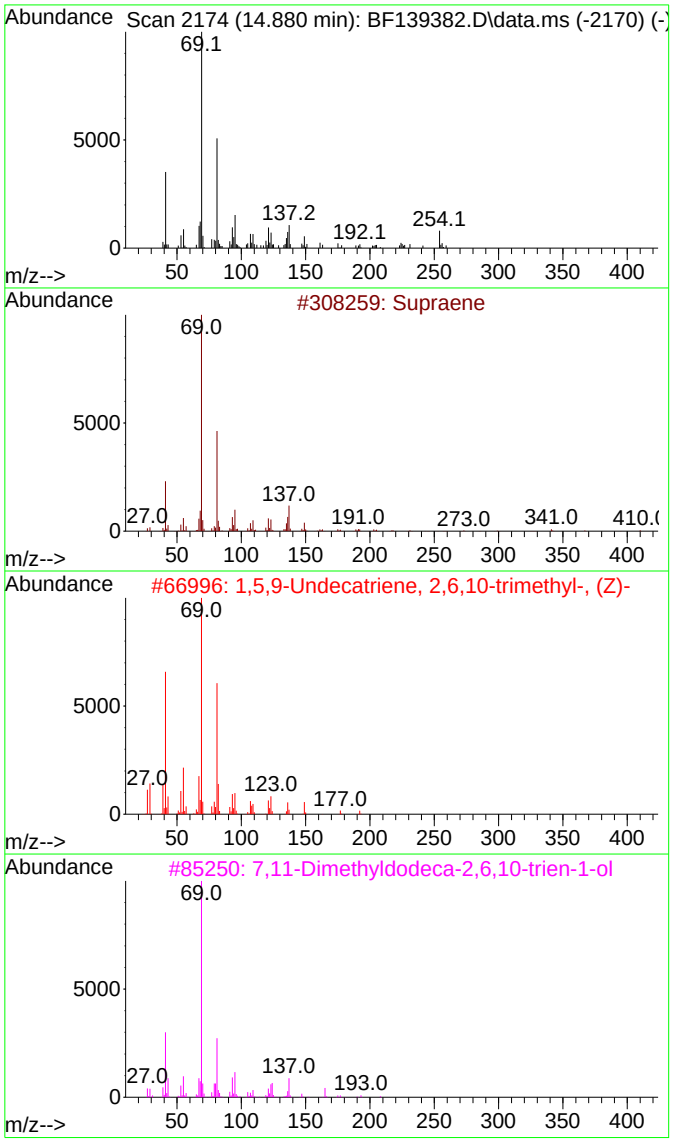
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

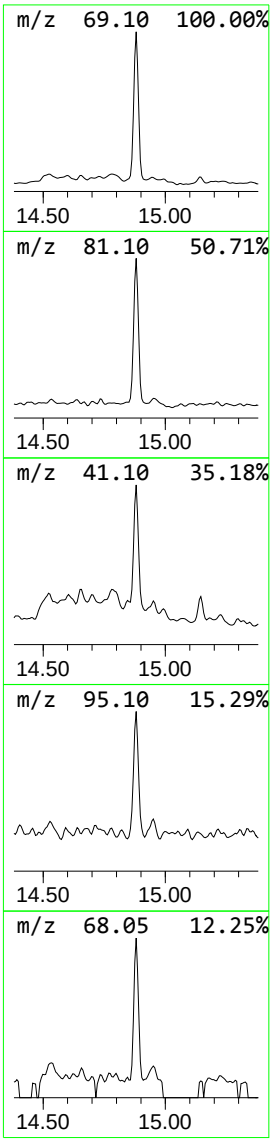
****

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	5.53 ng	80011	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	64





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Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

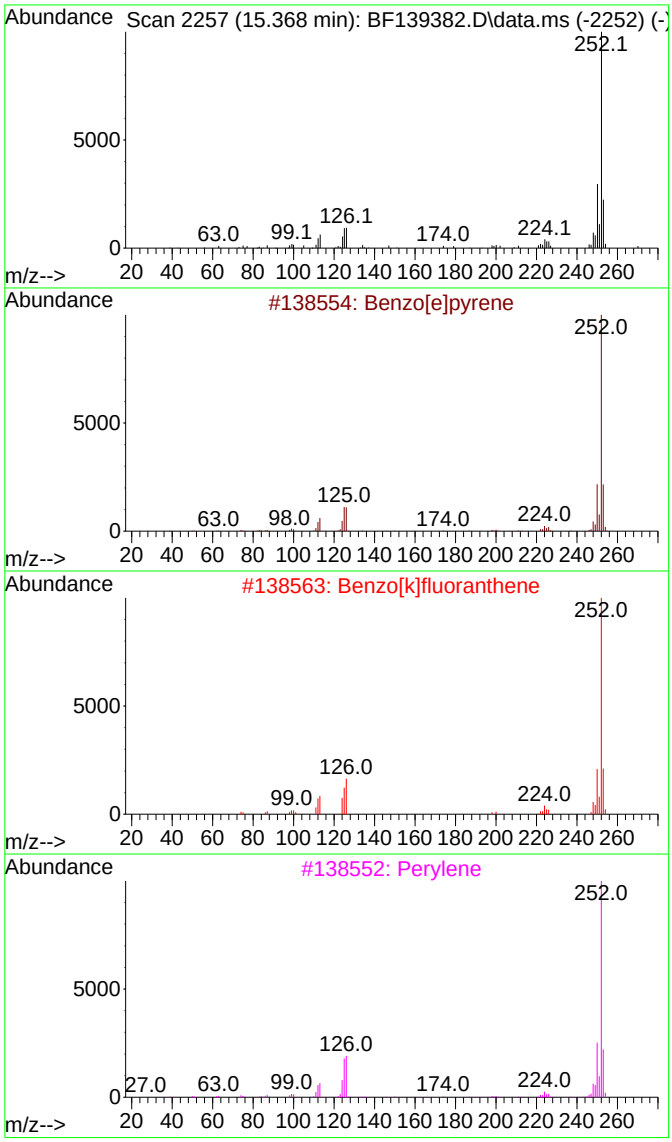
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

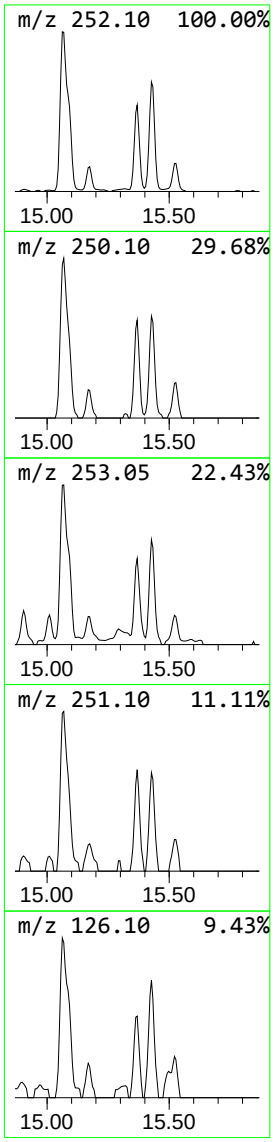
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	4.62 ng	66839	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139382.D
Acq On : 16 Sep 2024 16:58
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.205	65.4	ng	1257060	1	6.875	384352	20.0
2-Pentanone, 4-...	5.099	5.5	ng	104687	1	6.875	384352	20.0
Benzophenone	10.622	5.4	ng	140315	3	9.910	520607	20.0
n-Hexadecanoic ...	11.922	11.1	ng	354755	4	11.392	637199	20.0
Heptadecyl hept...	13.874	4.2	ng	119078	5	14.027	571398	20.0
Supraene	14.880	5.5	ng	80011	6	15.492	289498	20.0
Benzo[e]pyrene	15.368	4.6	ng	66839	6	15.492	289498	20.0