LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-W-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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	21	rVB	2098618	2562834	77.10%	8.919%
2	2.281	29	33	39	rVB	33172	44283	1.33%	0.154%
3	3.399	220	223	234	rBV	79438	165548	4.98%	0.576%
4	5.093	508	511	520	rVB	294903	339348	10.21%	1.181%
5	5.504	576	581	584	rBV	3534468	3283214	98.78%	11.426%
6	5.822	630	635	641	rBV	48909	46380	1.40%	0.161%
7	6.510	747	752	755	rBV	3696825	3323882	100.00%	11.567%
8	6.698	781	784	787	rBV	103319	82027	2.47%	0.285%
9	6.875	810	814	817	rBV	1527790	1244005	37.43%	4.329%
10	6.934	819	824	828	rVB	48940	41056	1.24%	0.143%
11	7.434	898	909	912	rBV	2370601	2133456	64.19%	7.424%
12	7.686	948	952	959	rVB	161169	125892	3.79%	0.438%
13	8.151	1028	1031	1034	rBV	1732381	1509134	45.40%	5.252%
14	8.369	1063	1068	1075	rVB	49122	45132	1.36%	0.157%
15	8.463	1081	1084	1088	rBV	253347	207515	6.24%	0.722%
16	9.228	1210	1214	1217	rBV	3589840	2767533	83.26%	9.631%
17	9.904	1326	1329	1333	rBV	1615902	1367279	41.14%	4.758%
18	9.939	1333	1335	1338	rVB	51939	41021	1.23%	0.143%
19	10.004	1341	1346	1351	rVB	104997	140359	4.22%	0.488%
20	10.692	1459	1463	1470	rBV	1642400	1375496	41.38%	4.787%
21	10.798	1478	1481	1487	rVB2	155023	161751	4.87%	0.563%
22	11.251	1552	1558	1560	rBV3	32571	35834	1.08%	0.125%
23	11.392	1578	1582	1584	rBV	1275691	1085376	32.65%	3.777%
24	11.416	1584	1586	1589	rVV	267228	219158	6.59%	0.763%
25	11.463	1589	1594	1597	rVB	81062	78869	2.37%	0.274%
26	11.622	1615	1621	1626	rBV	28899	40546	1.22%	0.141%
27	11.916	1668	1671	1677	rBV2	187026	181107	5.45%	0.630%
28	12.004	1683	1686	1688	rBV2	58100	58792	1.77%	0.205%
29	12.439	1757	1760	1763	rBV	32565	35966	1.08%	0.125%
30	12.474	1763	1766	1771	rVB2	32108	39987	1.20%	0.139%
31	12.598	1784	1787	1791	rBV	439302	384332	11.56%	1.337%
32	12.698	1801	1804	1807	rBV	71074	82875	2.49%	0.288%
33	12.827	1821	1826	1832	rVB	390721	399935	12.03%	1.392%
34	12.974	1847	1851	1854	rBV	2203601	1940875	58.39%	6.754%
35	13.051	1859	1864	1867	rBV3	30128	51432	1.55%	0.179%
36	13.157	1879	1882	1884	rVB	58436	49009	1.47%	0.171%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.221	1891	1893	1896	rVB	47513	37413	1.13%	0.130%
38	13.263	1896	1900	1902	rBV2	45316	50647	1.52%	0.176%
39	13.545	1945	1948	1952	rBV2	32151	39394	1.19%	0.137%
40	13.868	1999	2003	2012	rVB	217788	268078	8.07%	0.933%
41	14.027	2025	2030	2032	rBV2	1167581	1190051	35.80%	4.141%
42	14.051	2032	2034	2041	rVB	197310	174667	5.25%	0.608%
43	14.186	2055	2057	2061	rVB	48258	37033	1.11%	0.129%
44	14.492	2106	2109	2114	rBV3	75669	130630	3.93%	0.455%
45	15.062	2203	2206	2209	rBV	127195	178632	5.37%	0.622%
46	15.139	2216	2219	2222	rBV	64207	64100	1.93%	0.223%
47	15.427	2265	2268	2274	rVB	107279	123797	3.72%	0.431%
48	15.492	2275	2279	2283	rBV	605138	749963	22.56%	2.610%

Sum of corrected areas: 28735643

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
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Sample : P3077-04
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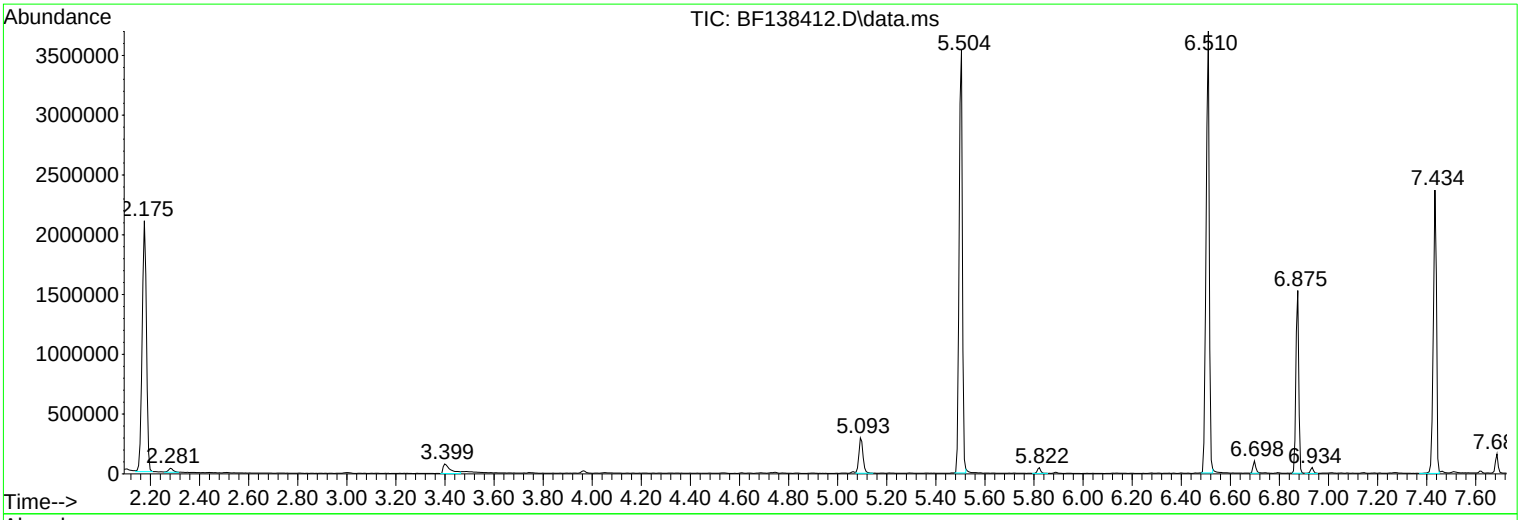
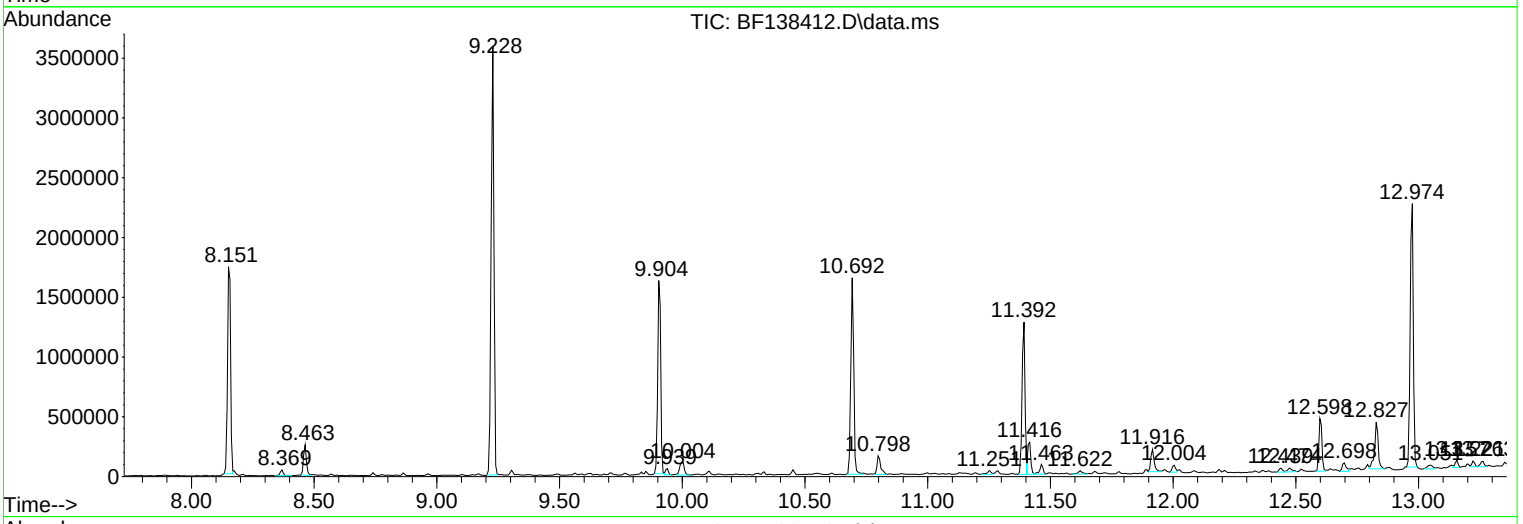
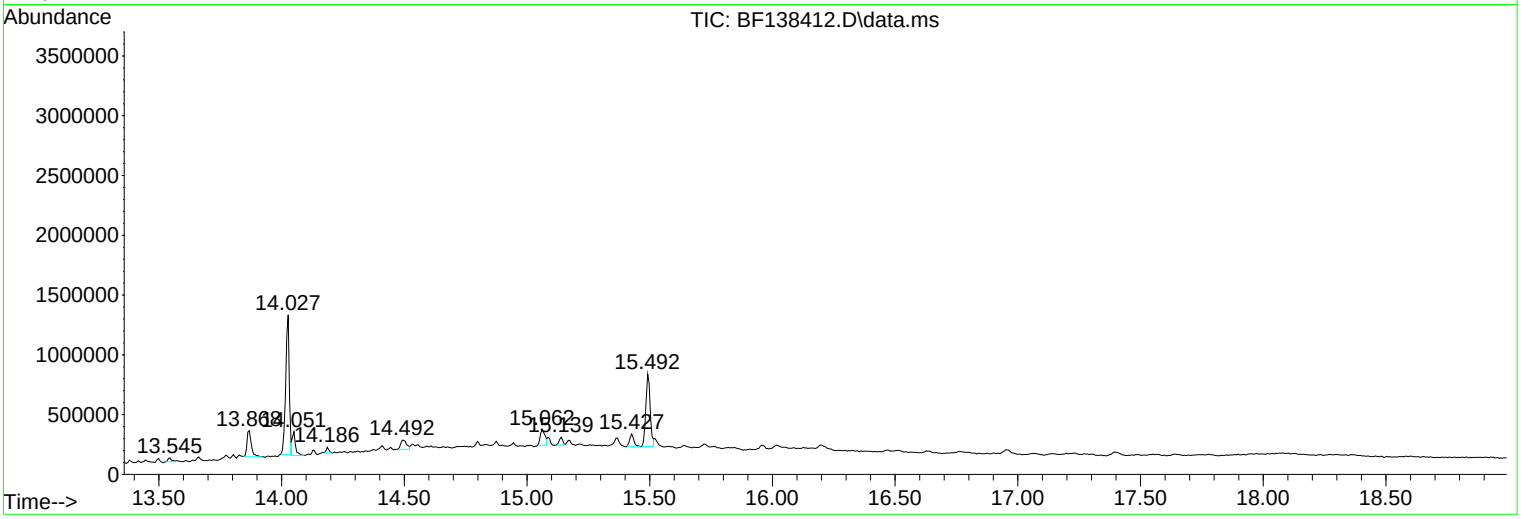
Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

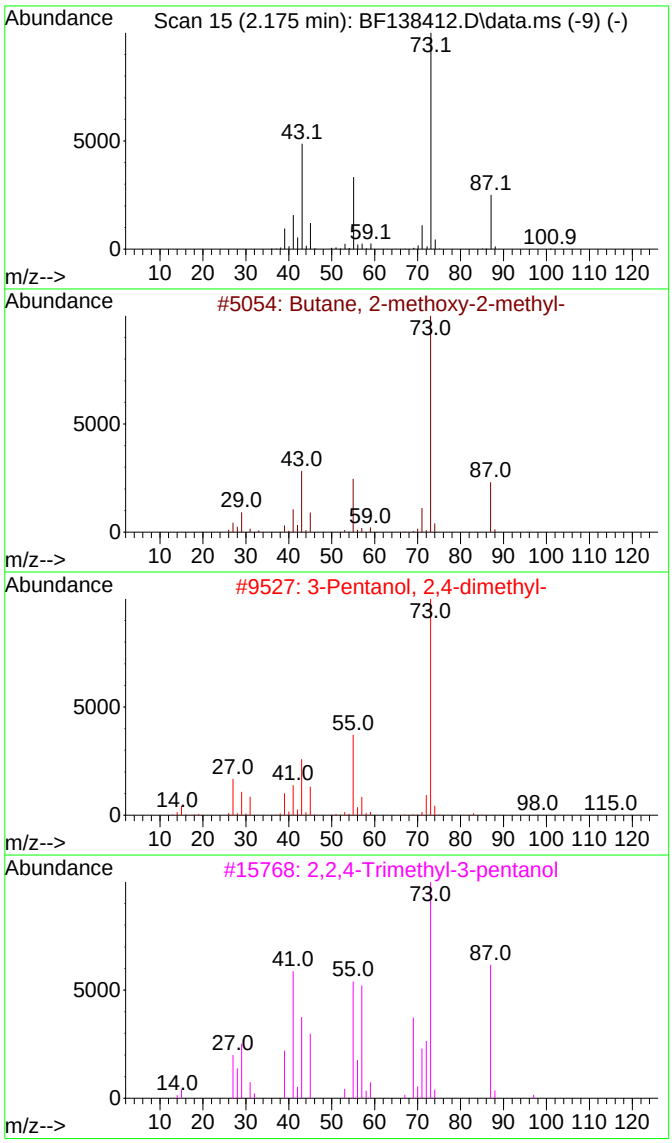
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

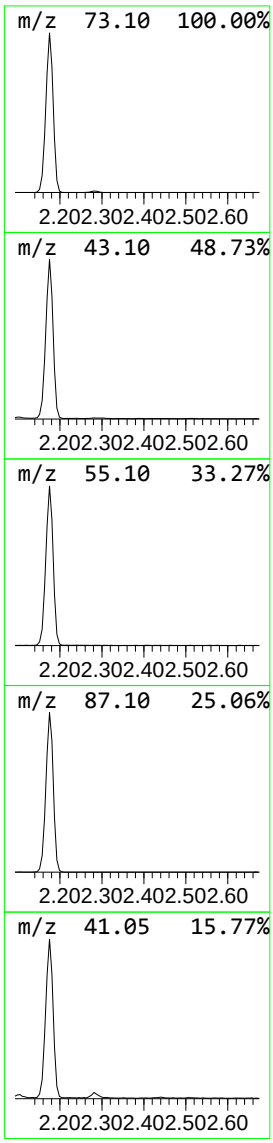
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	41.20 ng	2562830	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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

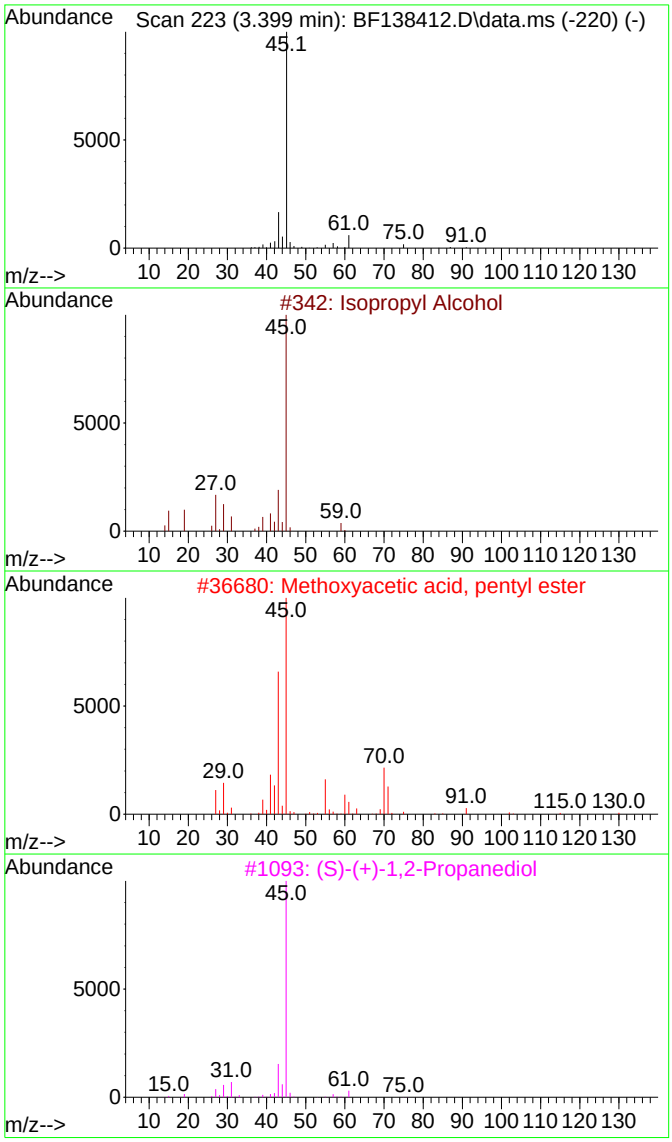
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

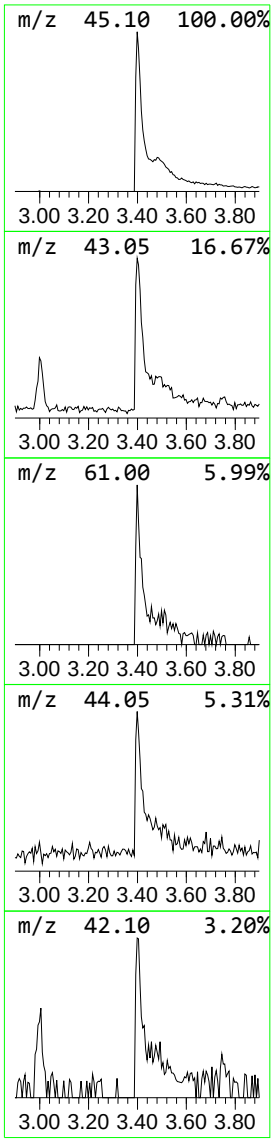
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	2.66 ng	165548	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
2	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	2,3-Butanediol	90	C4H10O2	000513-85-9	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

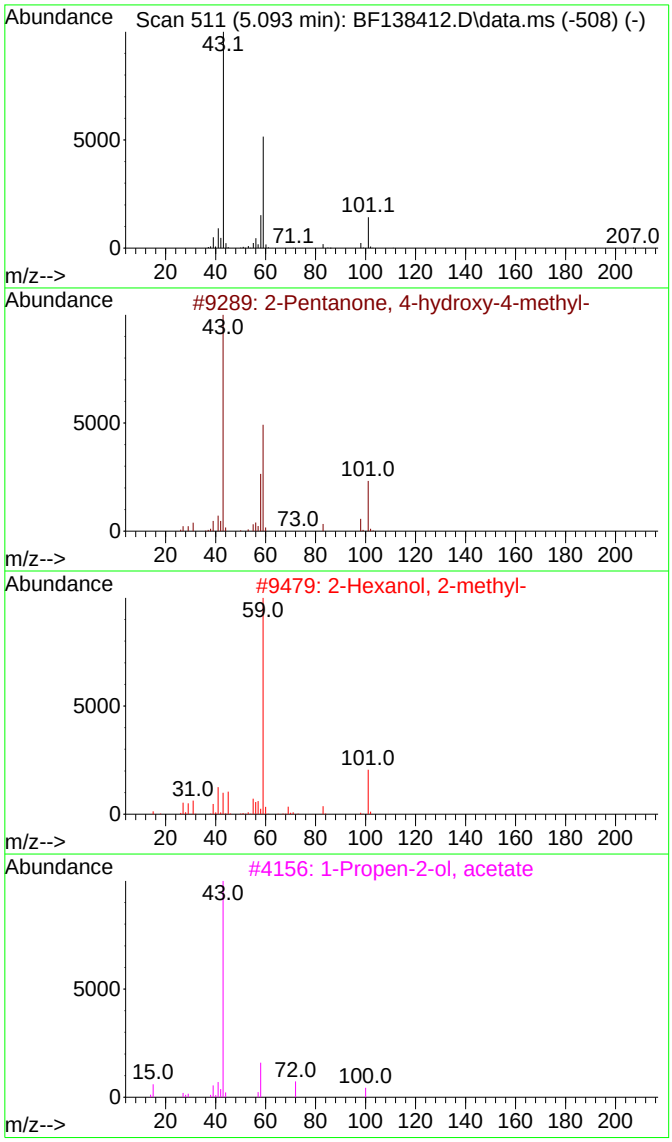
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

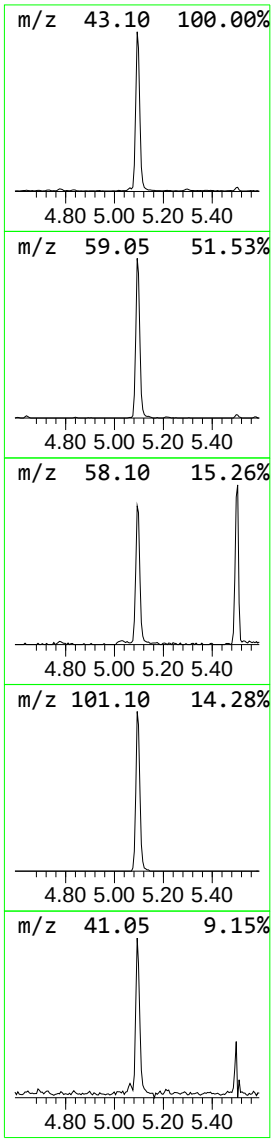
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	5.46 ng	339348	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	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

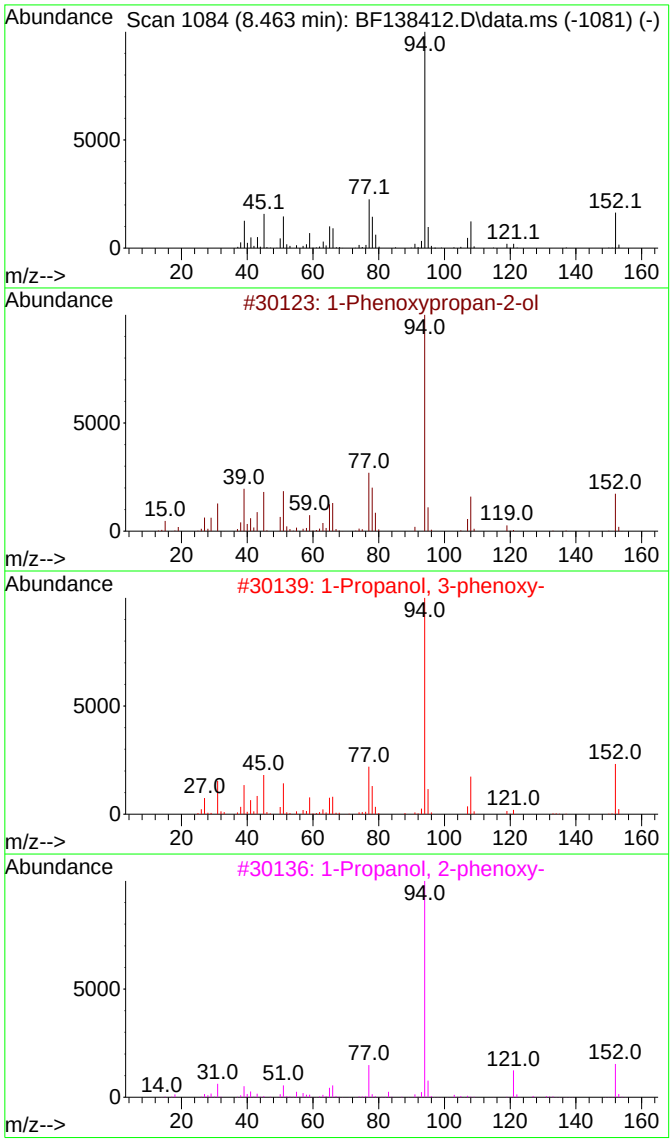
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

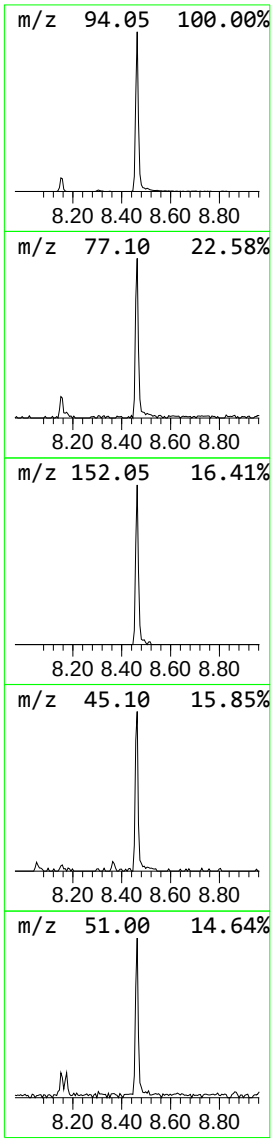
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.75 ng	207515	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
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Operator : CG\JU
Sample : P3077-04
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Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

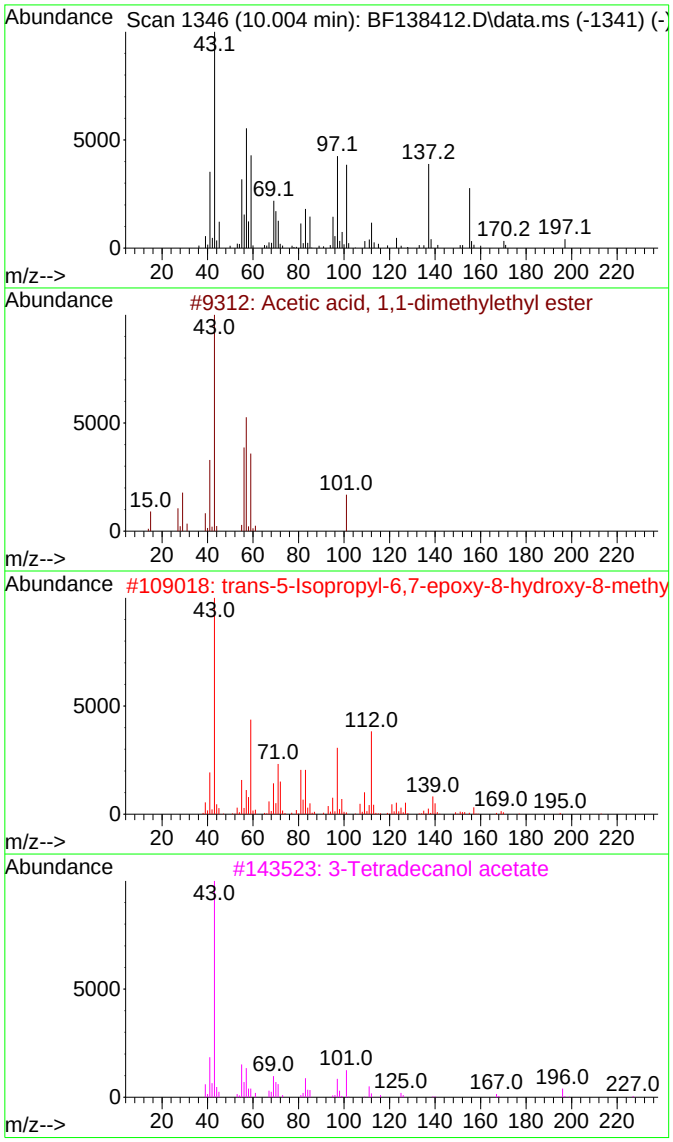
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

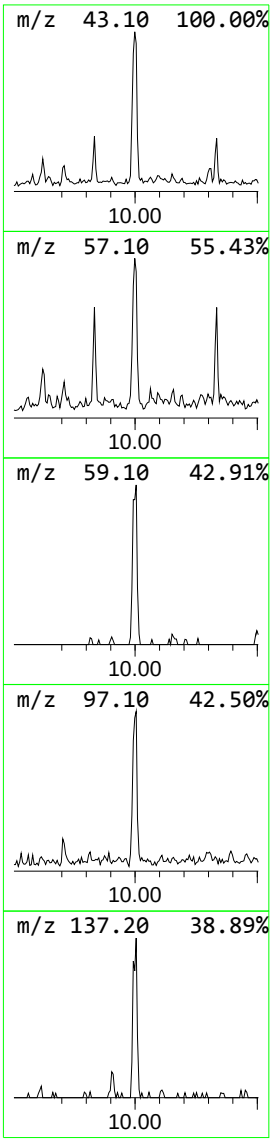
****

Peak Number 5 unknown10.004 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	2.05 ng	140359	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
3	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	12
4	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	9





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

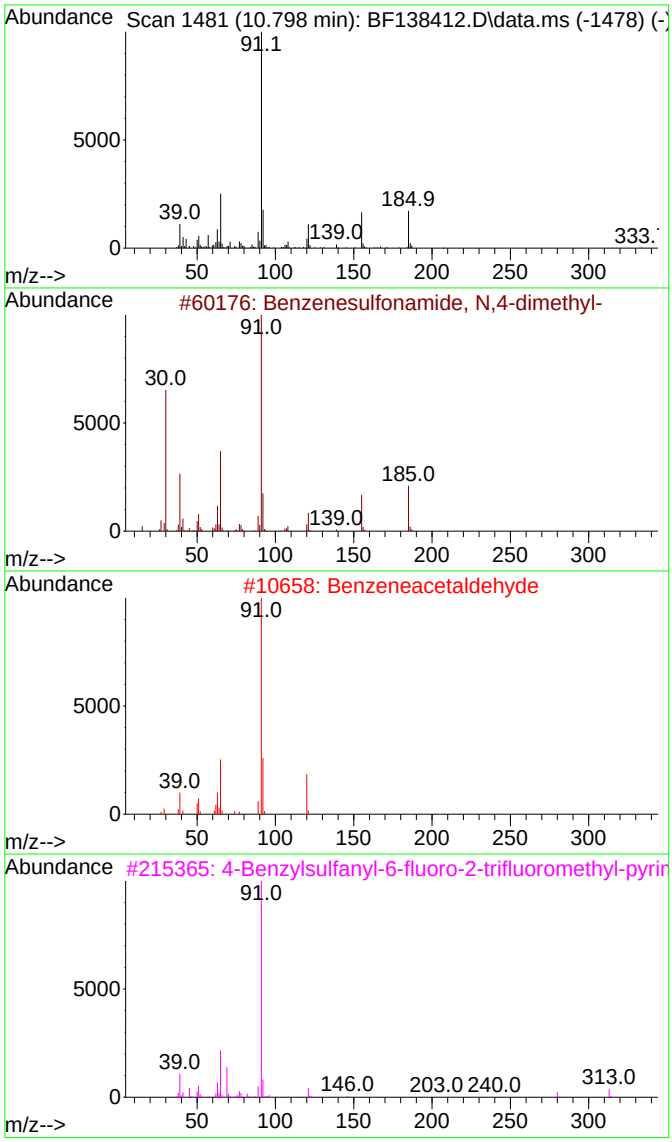
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

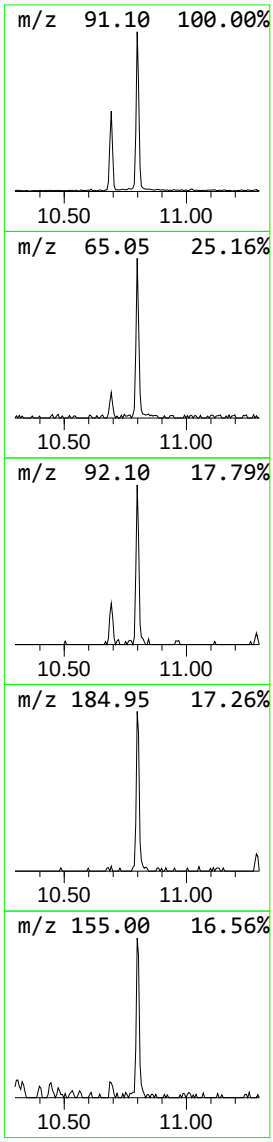
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	2.98 ng	161751	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	96
2	Benzeneacetaldehyde	120	C8H8O	000122-78-1	60
3	4-Benzylsulfanyl-6-fluoro-2-trif...	313	C13H7F4N3S	1000296-93-7	47
4	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	46
5	Benzaldehyde, 2-methyl-	120	C8H8O	000529-20-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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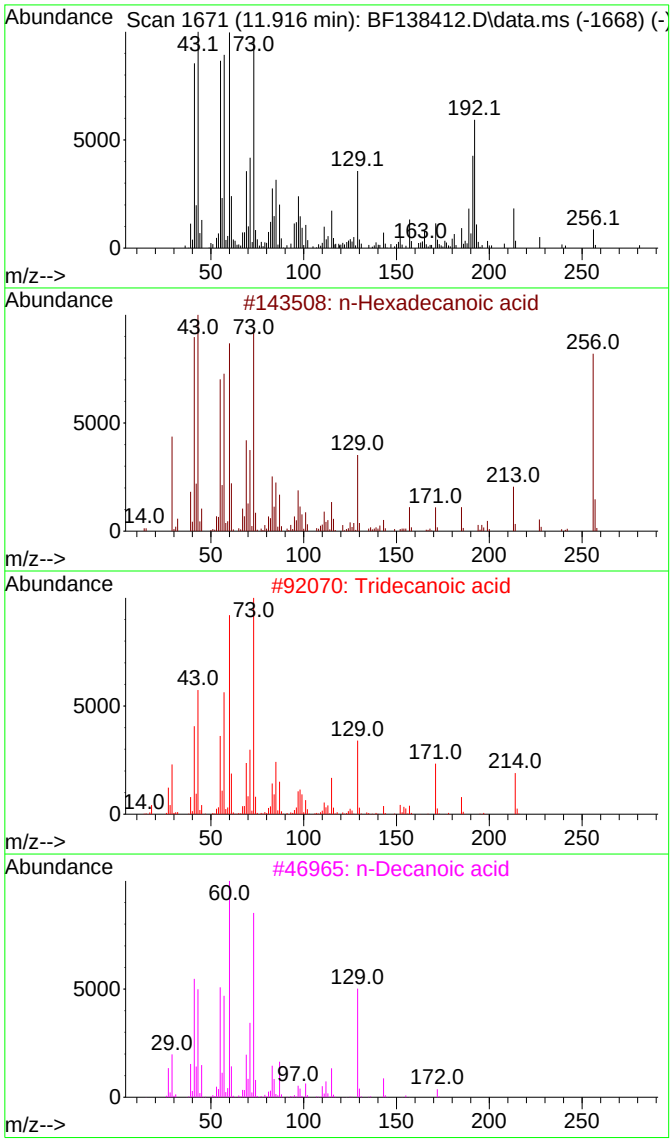
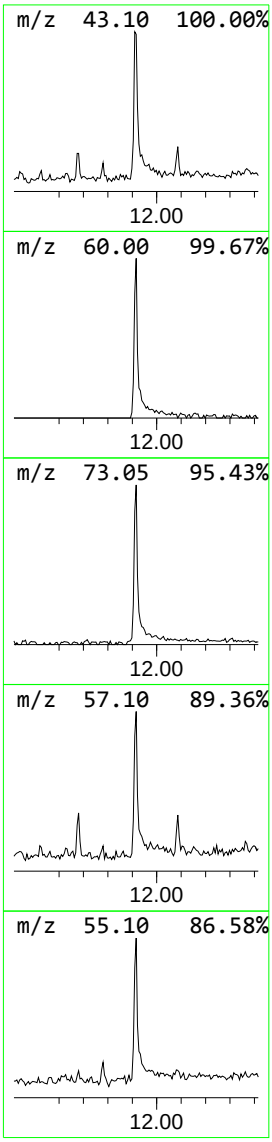
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.34 ng	181107	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	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	55
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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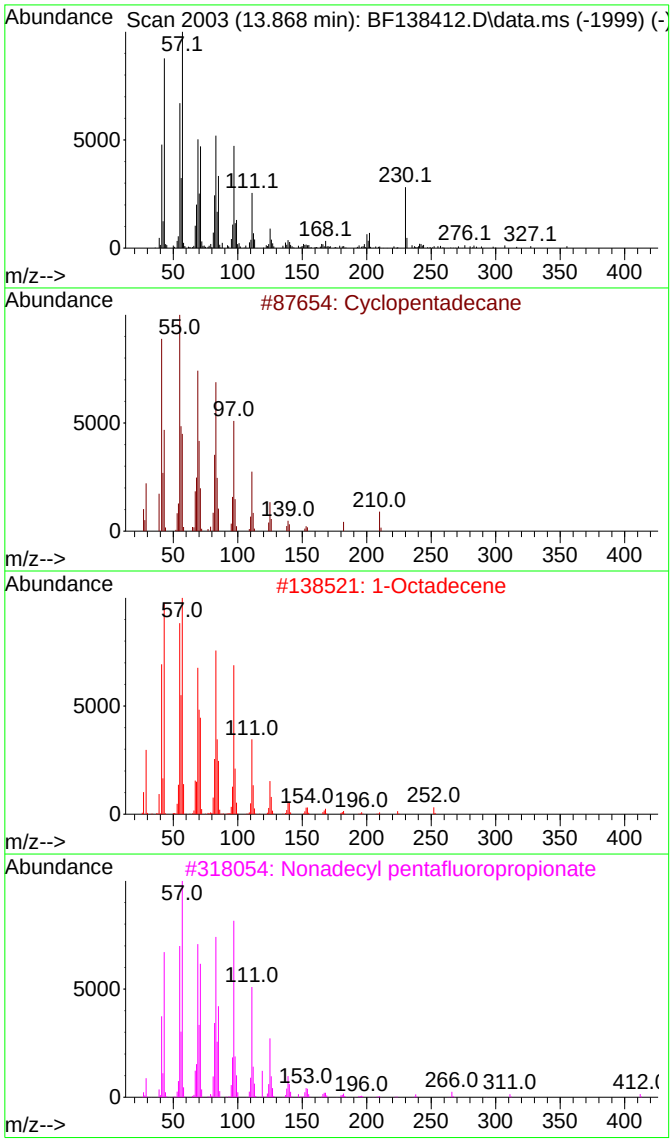
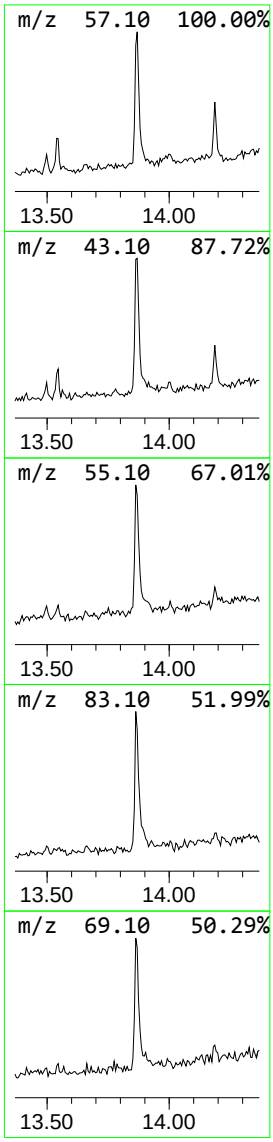
Peak Number 8 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	4.51 ng	268078	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	1-Octadecene	252	C18H36	000112-88-9	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	87
5	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

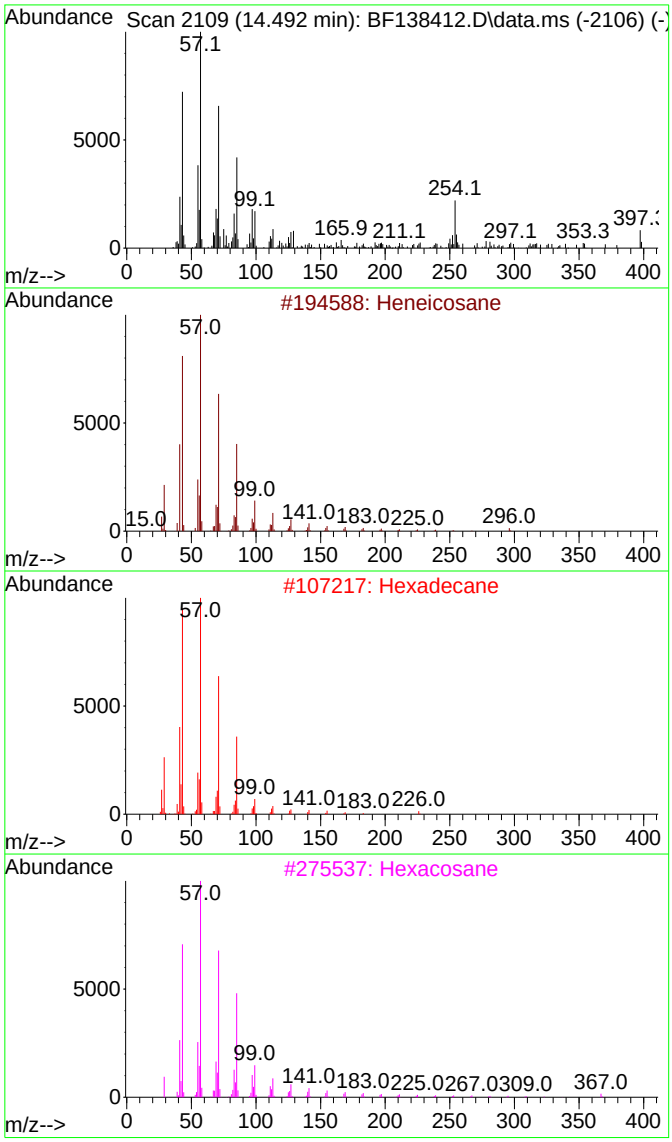
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

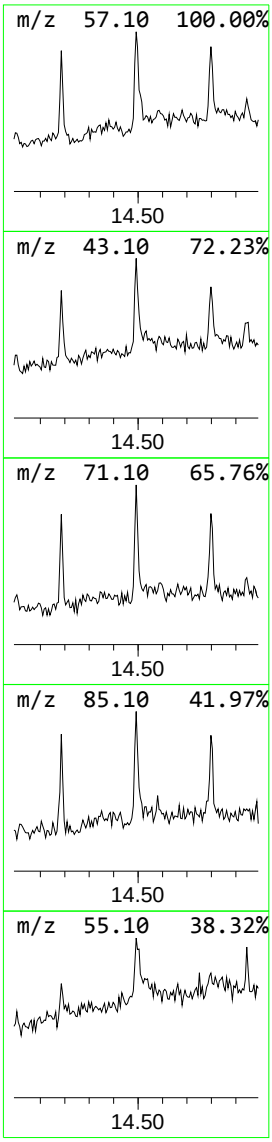
****

Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.20 ng	130630	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	92
2	Hexadecane	226	C16H34	000544-76-3	86
3	Hexacosane	366	C26H54	000630-01-3	76
4	Heptacosane	380	C27H56	000593-49-7	76
5	Heptadecane	240	C17H36	000629-78-7	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138412.D
Acq On : 01 Jul 2024 19:35
Operator : CG\JU
Sample : P3077-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-W-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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...	2.175	41.2	ng	2562830	1	6.875	1244010	20.0
Isopropyl Alcohol	3.399	2.7	ng	165548	1	6.875	1244010	20.0
2-Pentanone, 4-...	5.093	5.5	ng	339348	1	6.875	1244010	20.0
1-Phenoxypropan...	8.463	2.8	ng	207515	2	8.151	1509130	20.0
unknown10.004	10.004	2.0	ng	140359	3	9.904	1367280	20.0
Benzenesulfonam...	10.798	3.0	ng	161751	4	11.392	1085380	20.0
n-Hexadecanoic ...	11.916	3.3	ng	181107	4	11.392	1085380	20.0
Cyclopentadecane	13.868	4.5	ng	268078	5	14.027	1190050	20.0
Heneicosane	14.492	2.2	ng	130630	5	14.027	1190050	20.0