LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080125\
Data File : BF143284.D
Acq On : 01 Aug 2025 16:03
Operator : RC/JU
Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

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-BF071725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	12	20	29	rVB	2072497	3425335	99.25%	13.328%
2	4.110	284	326	339	rBV2	52659	368341	10.67%	1.433%
3	4.687	372	424	432	rBV	97415	900987	26.11%	3.506%
4	5.193	503	510	514	rBV	177695	269703	7.81%	1.049%
5	5.369	514	540	543	rBV	111295	619918	17.96%	2.412%
6	5.522	551	566	572	rVB2	109606	440017	12.75%	1.712%
7	5.593	572	578	594	rVB	1226369	1618377	46.89%	6.297%
8	5.757	594	606	612	rBV	62167	175030	5.07%	0.681%
9	5.934	631	636	649	rBV	44719	76220	2.21%	0.297%
10	6.087	654	662	684	rVB2	18881	55795	1.62%	0.217%
11	6.251	684	690	698	rBV2	15807	37794	1.10%	0.147%
12	6.581	738	746	759	rBV	959079	1310807	37.98%	5.101%
13	6.957	805	810	816	rVB	593237	742701	21.52%	2.890%
14	7.516	891	905	910	rBV	1560148	2157309	62.51%	8.394%
15	7.957	974	980	999	rVB4	12402	37889	1.10%	0.147%
16	8.151	1008	1013	1023	rBV	43000	85205	2.47%	0.332%
17	8.239	1023	1028	1043	rVB	697445	892442	25.86%	3.473%
18	8.763	1107	1117	1125	rBV	23809	61816	1.79%	0.241%
19	8.934	1139	1146	1163	rVB	385535	695325	20.15%	2.706%
20	9.316	1205	1211	1216	rBV	2612784	3451290	100.00%	13.429%
21	9.445	1229	1233	1246	rVB2	21586	39485	1.14%	0.154%
22	9.992	1321	1326	1339	rVB	763044	975692	28.27%	3.797%
23	10.704	1442	1447	1452	rBV	125520	151798	4.40%	0.591%
24	10.781	1455	1460	1475	rBV	1320134	1837334	53.24%	7.149%
25	11.192	1524	1530	1549	rBV	260115	414915	12.02%	1.614%
26	11.480	1574	1579	1586	rBV	626307	781373	22.64%	3.040%
27	12.004	1662	1668	1684	rBV2	67706	129124	3.74%	0.502%
28	13.069	1843	1849	1854	rBV	2020775	2695982	78.12%	10.490%
29	14.016	2004	2010	2020	rBV6	12083	43531	1.26%	0.169%
30	14.121	2022	2028	2039	rVB	458556	601325	17.42%	2.340%
31	14.980	2170	2174	2187	rVB	40498	63173	1.83%	0.246%
32	15.627	2277	2284	2295	rBV	340903	543503	15.75%	2.115%

Sum of corrected areas: 25699536

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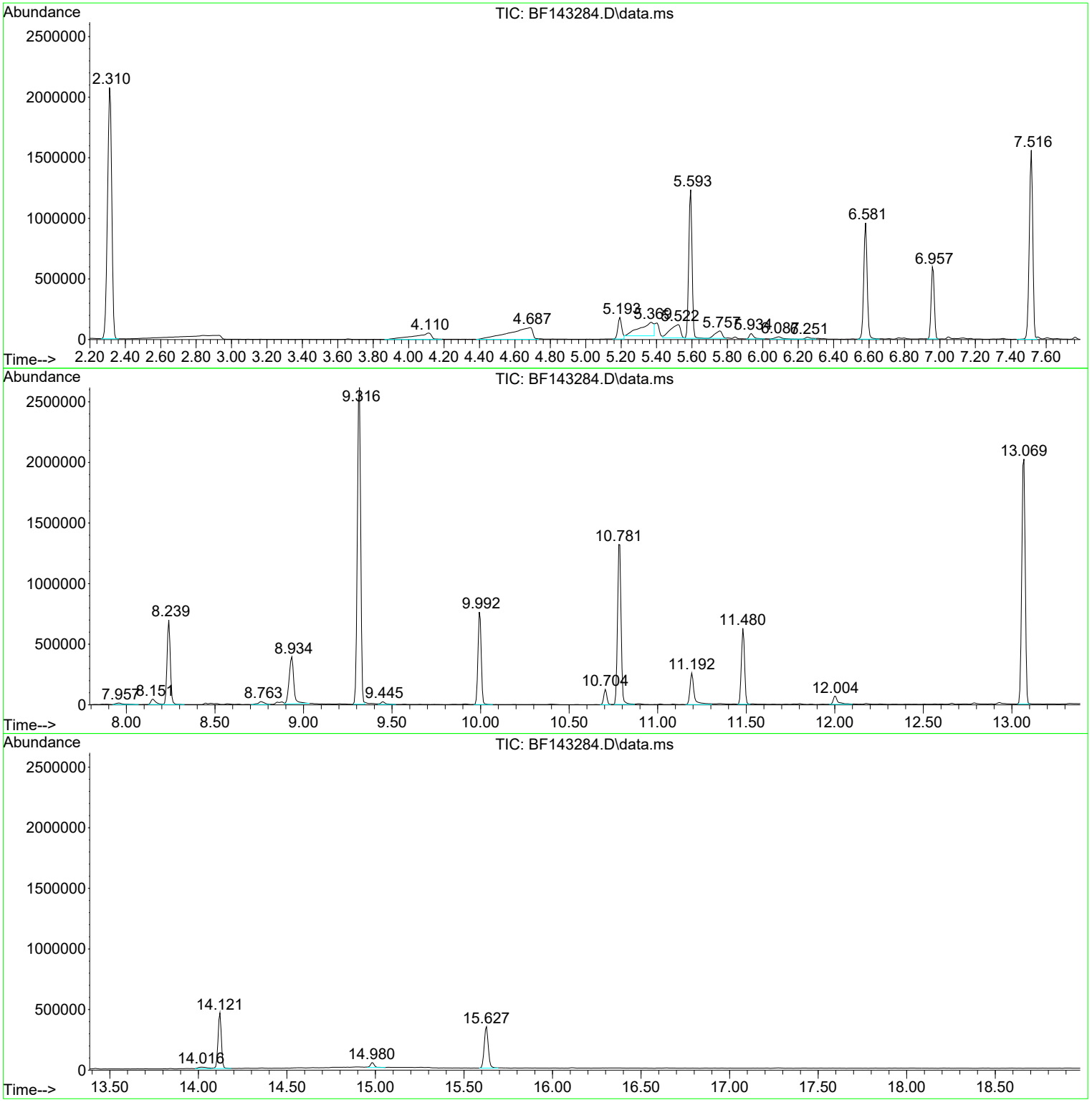
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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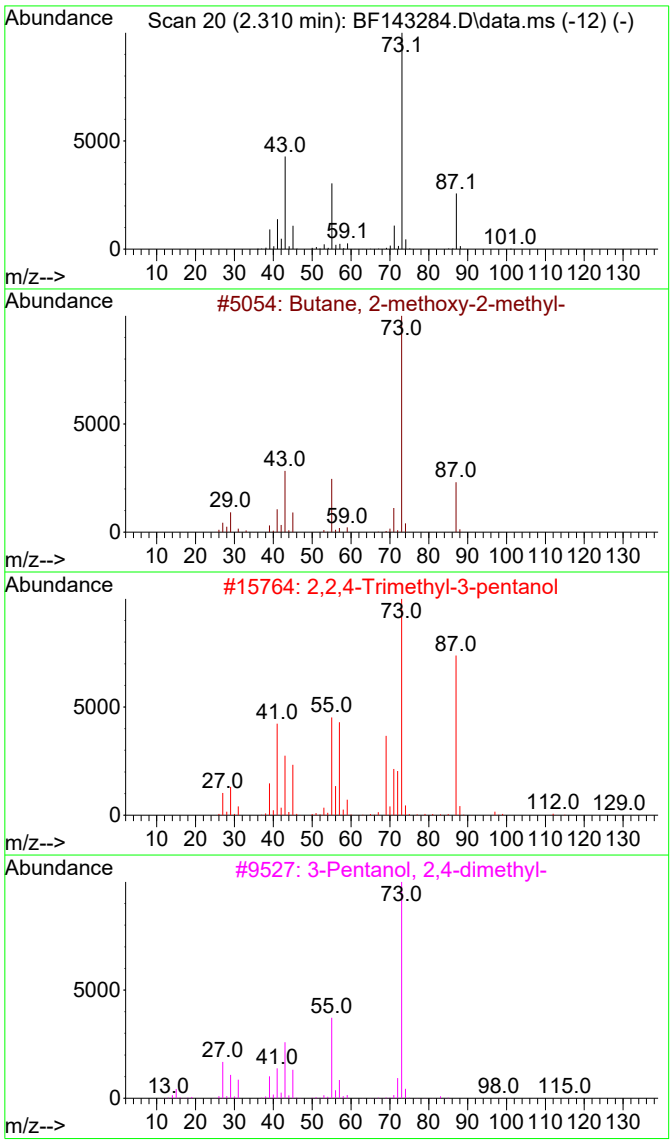
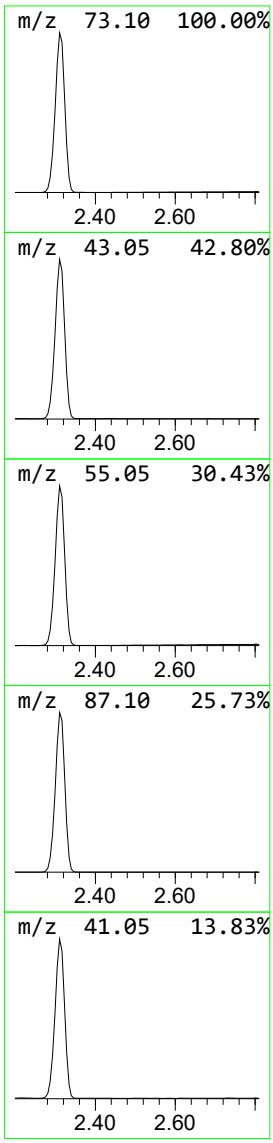
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.310	92.24 ng	3425340	1,4-Dichlorobenzene-d4	6.957

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Data File : BF143284.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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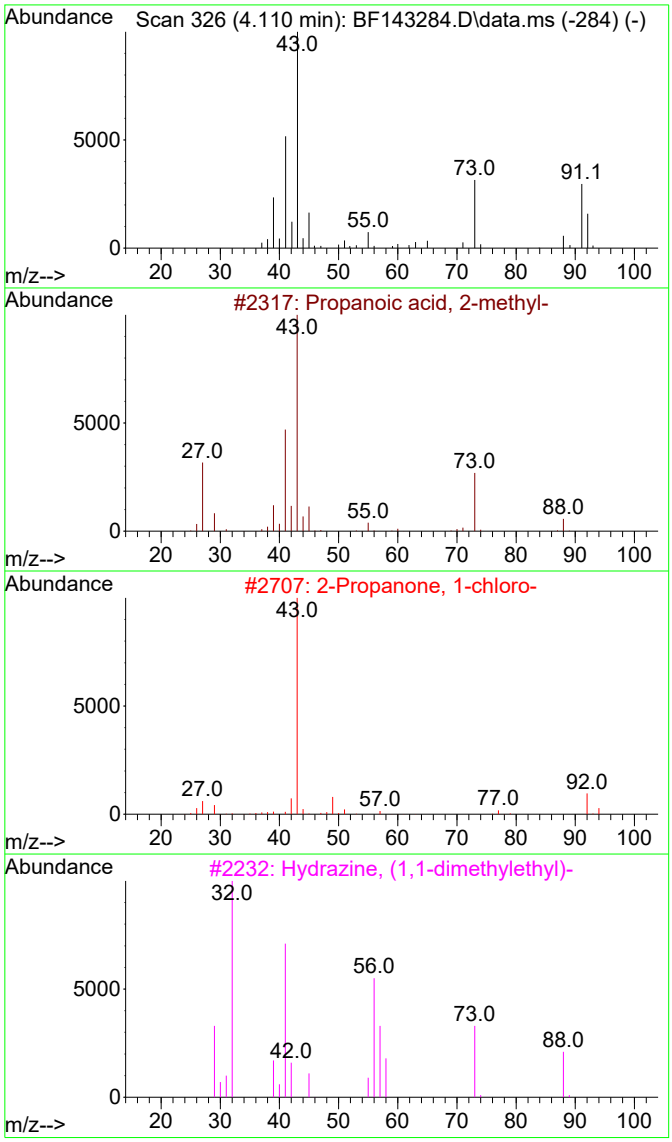
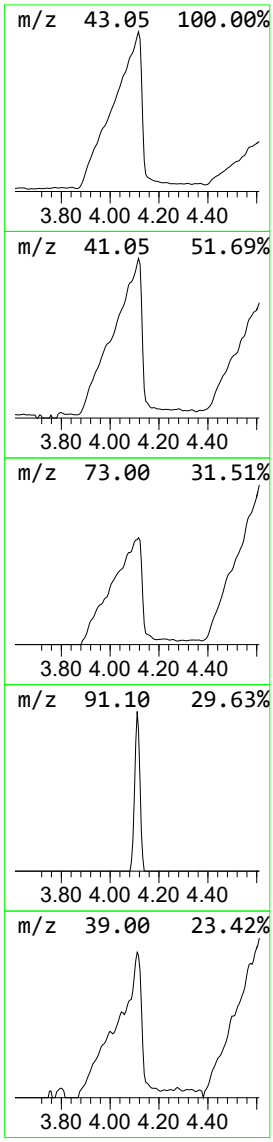
Peak Number 2 Propanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.110	9.92 ng	368341	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	68
2	2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	25
3	Hydrazine, (1,1-dimethylethyl)-	88	C4H12N2	032064-67-8	17
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	10
5	Butanenitrile, 3-methyl-	83	C5H9N	000625-28-5	9





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
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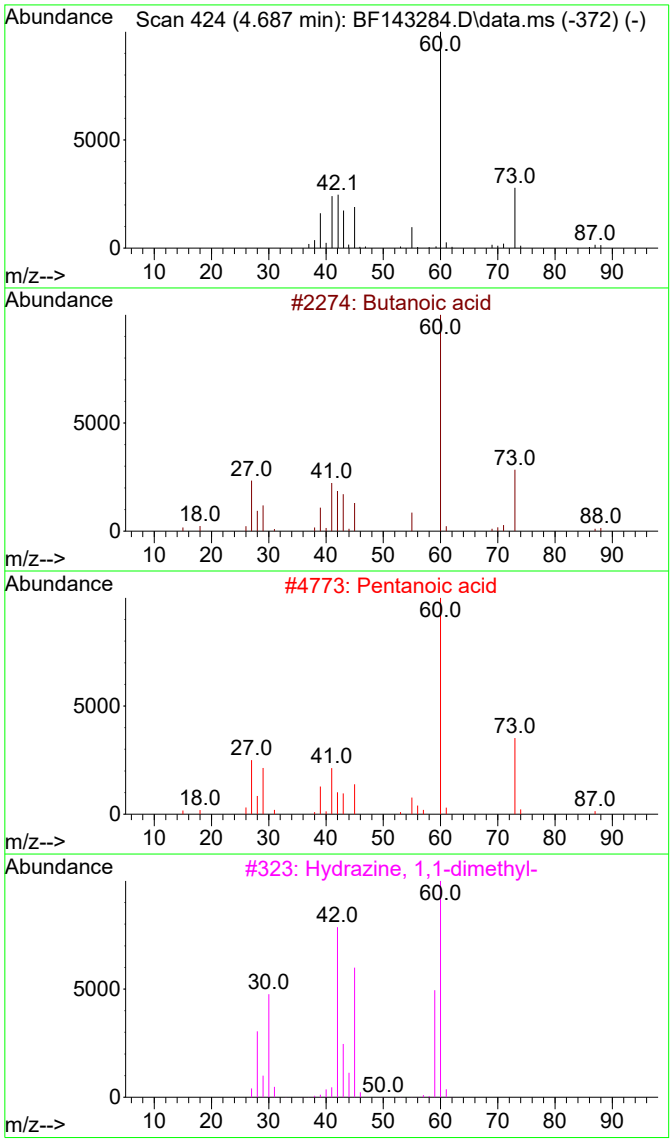
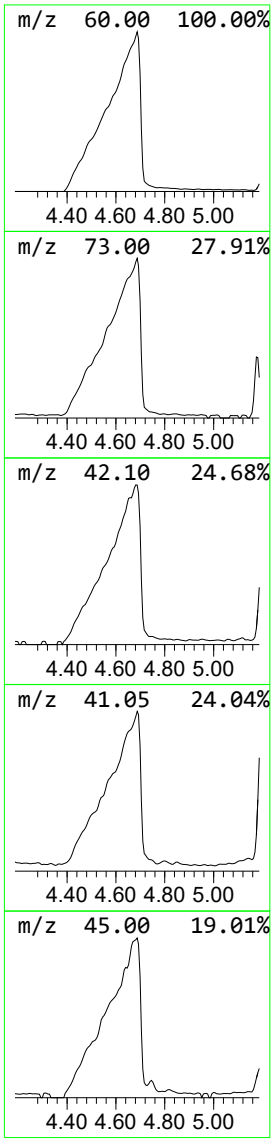
Peak Number 3 Butanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	24.26 ng	900987	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	90
2	Pentanoic acid	102	C5H10O2	000109-52-4	50
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Formamidoxime	60	CH4N2O	000624-82-8	9
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

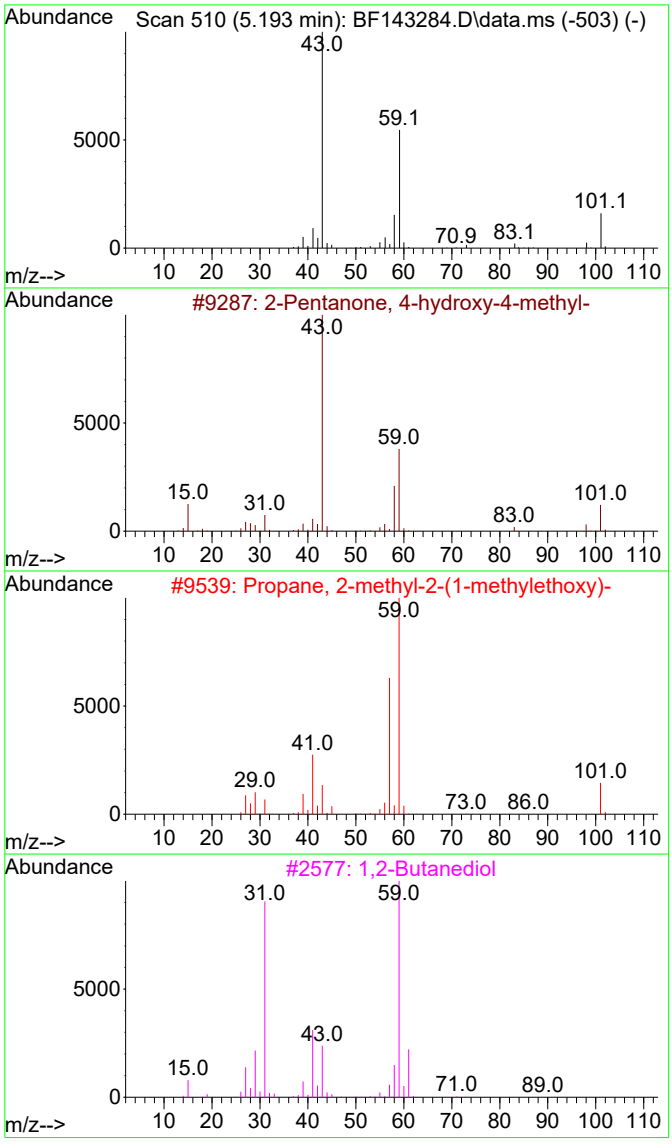
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

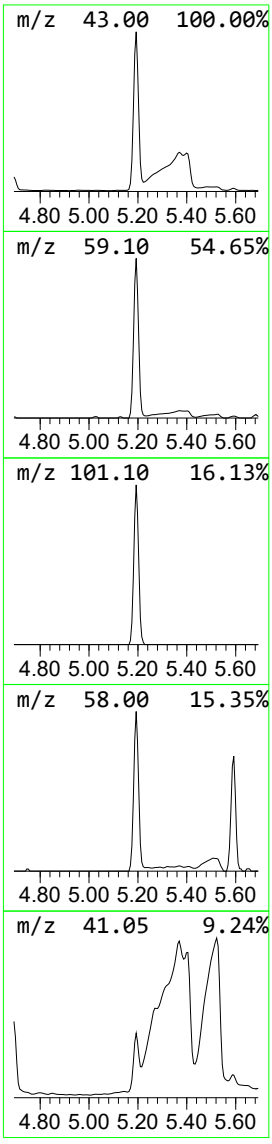
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	7.26 ng	269703	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	1,2-Butanediol	90	C4H10O2	000584-03-2	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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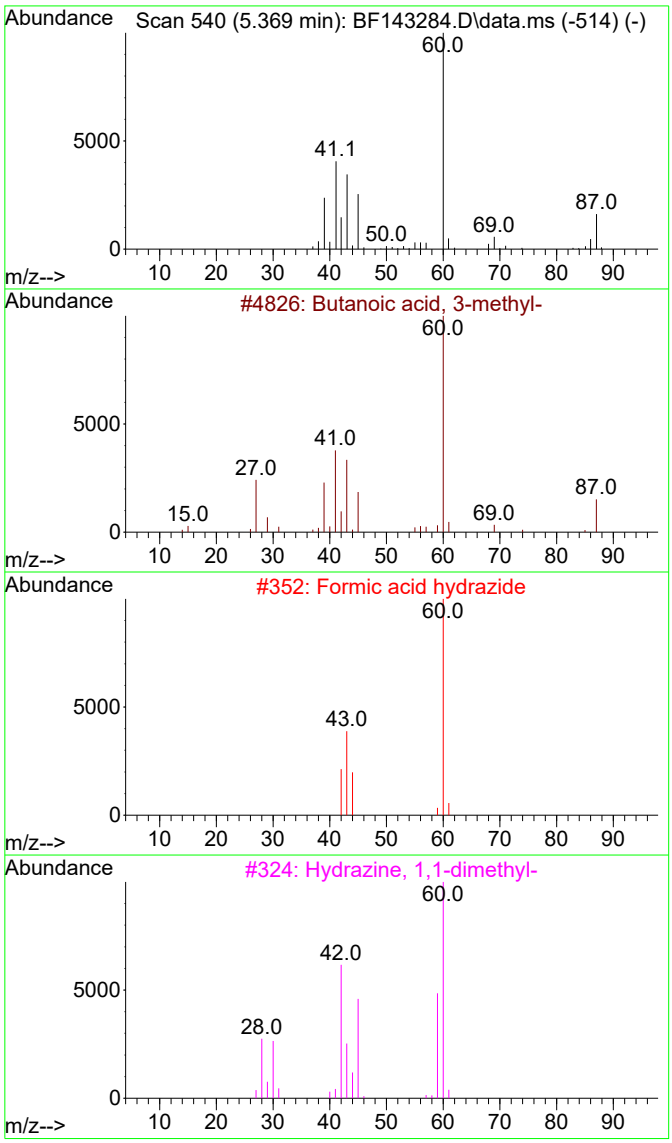
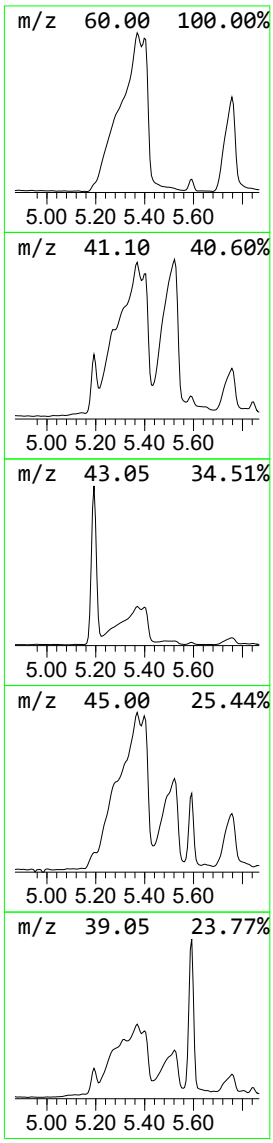
Peak Number 5 Butanoic acid, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.369	16.69 ng	619918	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	40
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	9





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BNA_F
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TIC Library : C:\Database\NIST20.L
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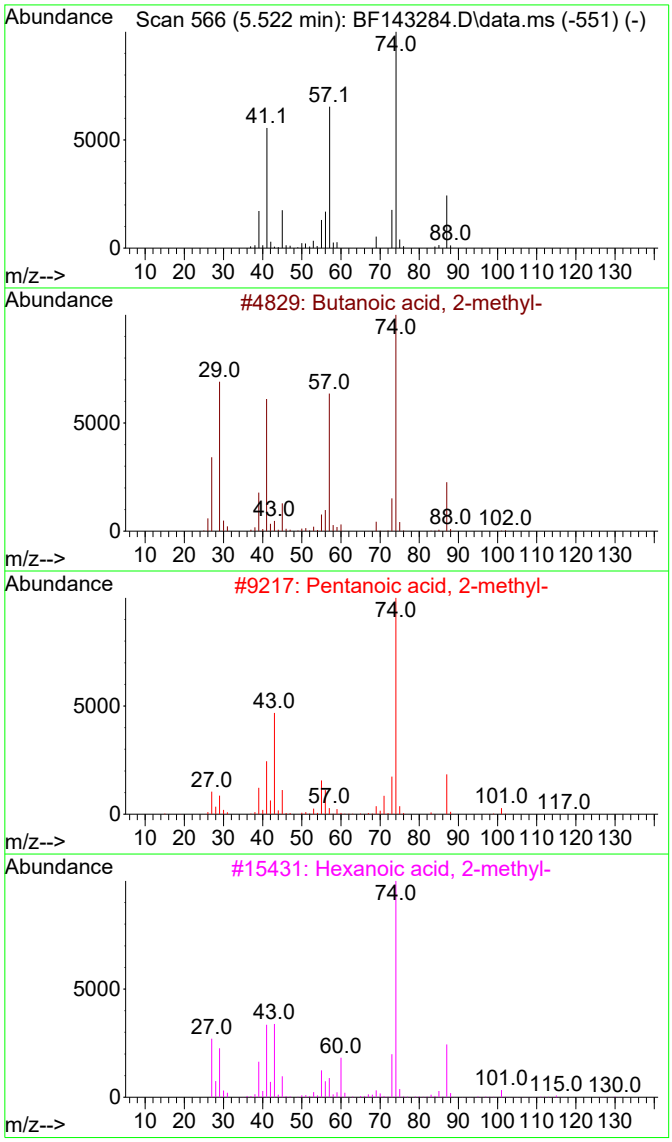
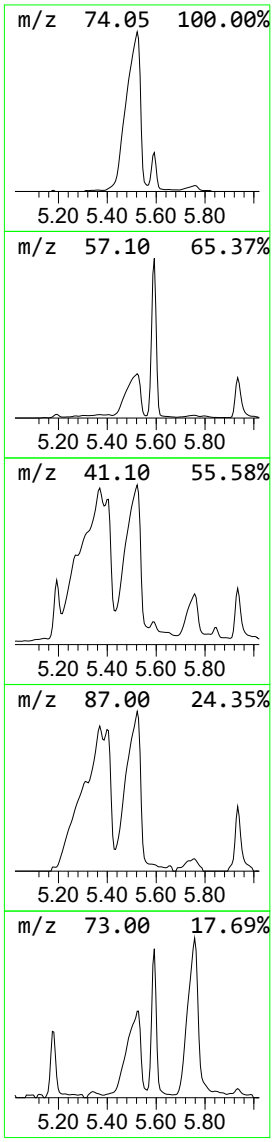
Peak Number 6 Butanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.522	11.85 ng	440017	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
3	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	50
4	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	10
5	Morpholine	87	C4H9NO	000110-91-8	9





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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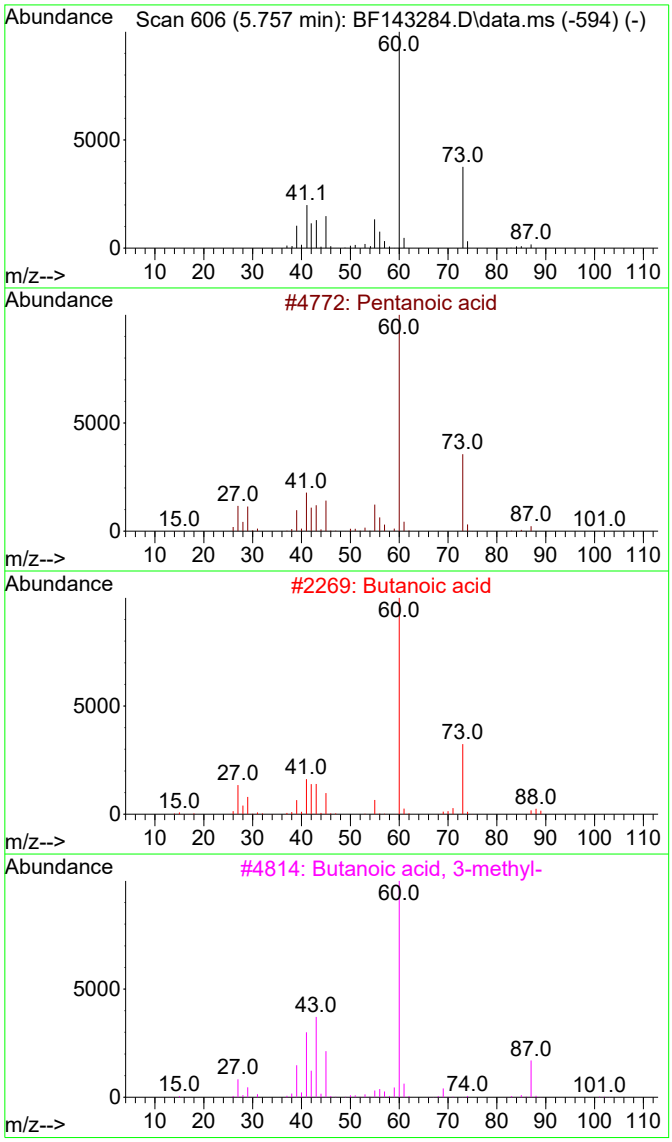
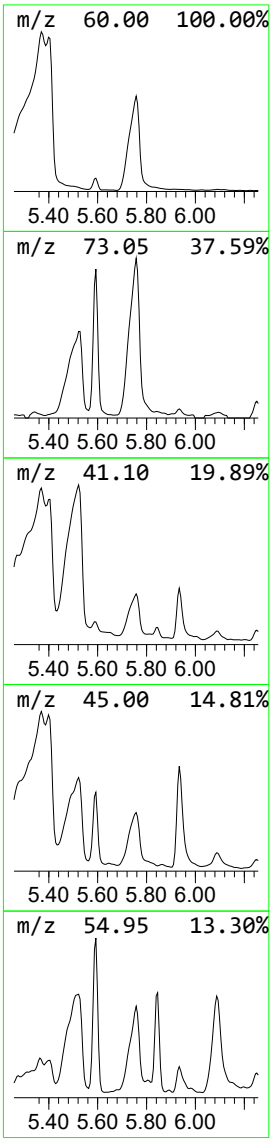
Peak Number 7 Pentanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.757	4.71 ng	175030	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	83
2	Butanoic acid	88	C4H8O2	000107-92-6	78
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	45
4	Hexanoic acid	116	C6H12O2	000142-62-1	43
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	42





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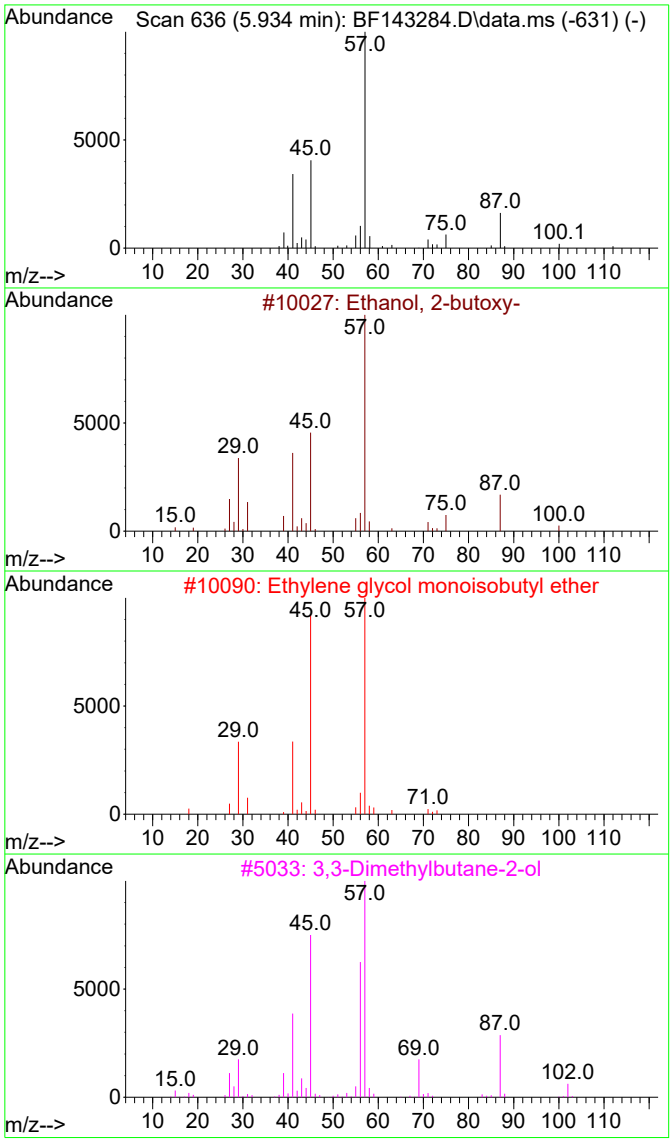
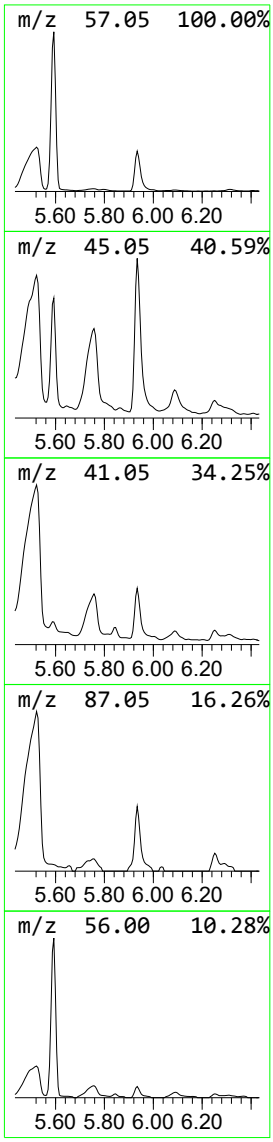
Peak Number 8 Ethanol, 2-butoxy- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.934	2.05 ng	76220	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38
4	n-Butyl ether	130	C8H18O	000142-96-1	35
5	Isobutyl ether	130	C8H18O	000628-55-7	25





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Sample : Q2733-01
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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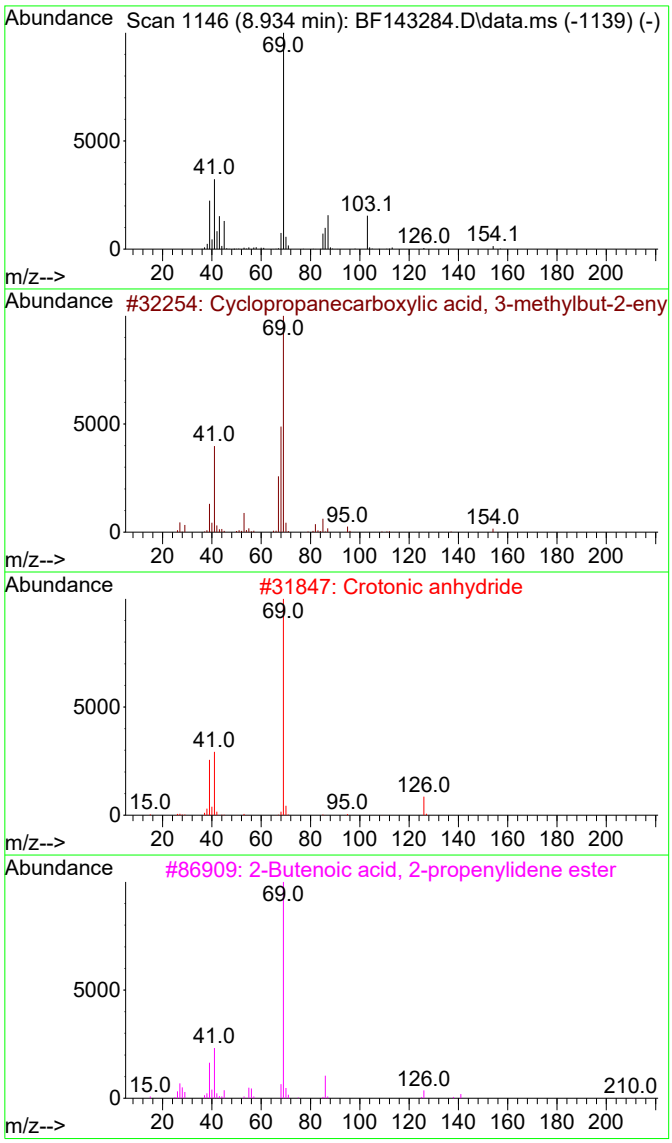
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

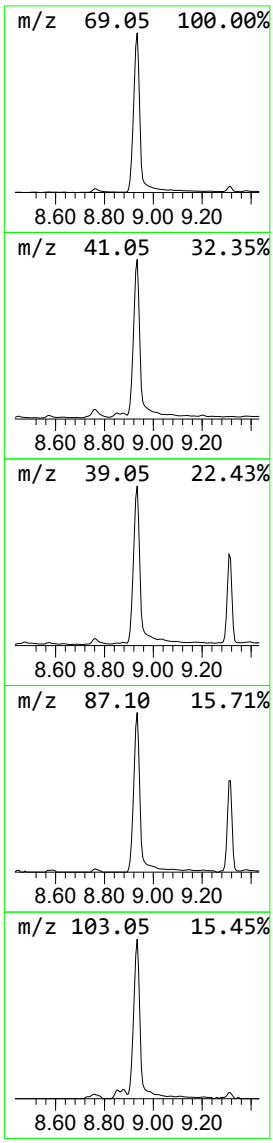
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopropanecarboxylic acid... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.934	15.58 ng	695325	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	50
2	Crotonic anhydride	154	C8H10O3	000623-68-7	47
3	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
4	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
5	1,6-Hexanediamine	116	C6H16N2	000124-09-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080125\
Data File : BF143284.D
Acq On : 01 Aug 2025 16:03
Operator : RC/JU
Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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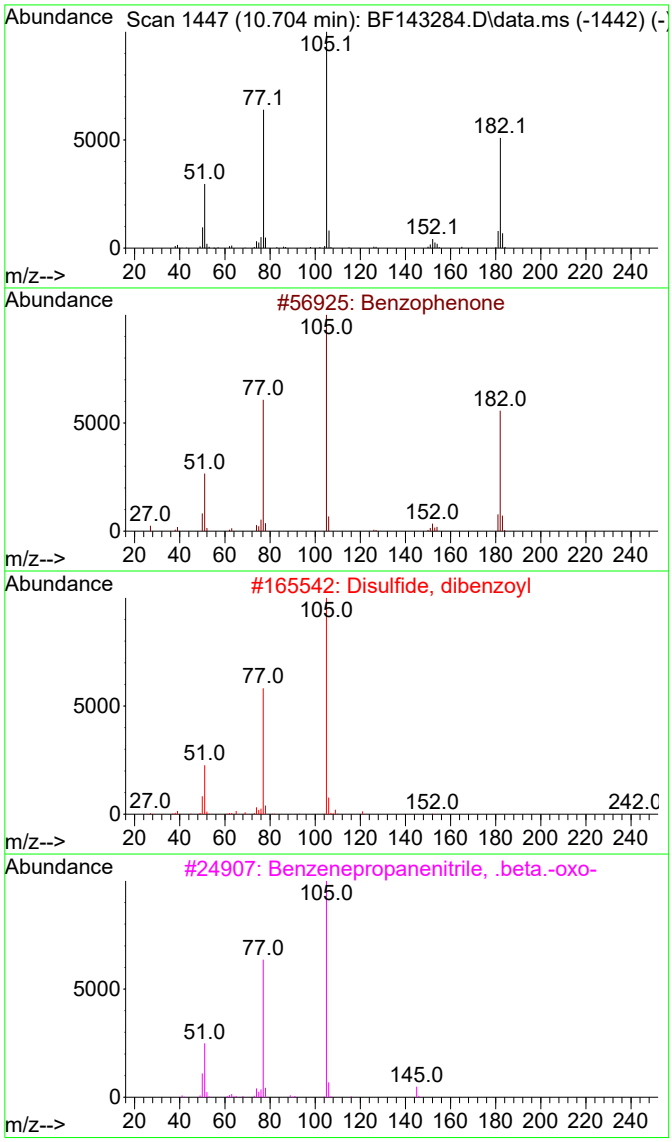
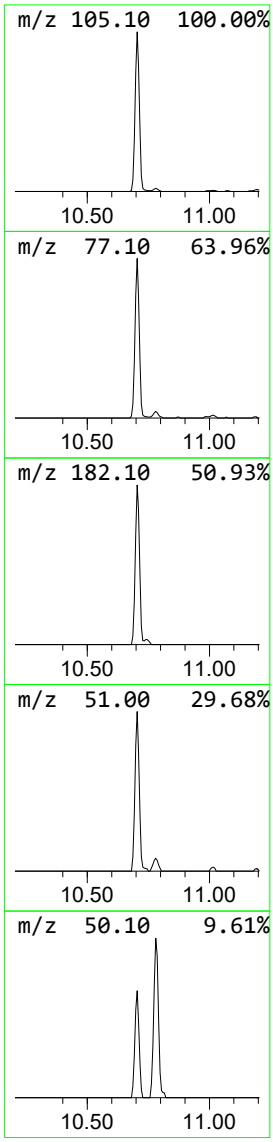
Peak Number 10 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	3.11 ng	151798	Acenaphthene-d10	9.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	50





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Misc :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
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TIC Library : C:\Database\NIST20.L
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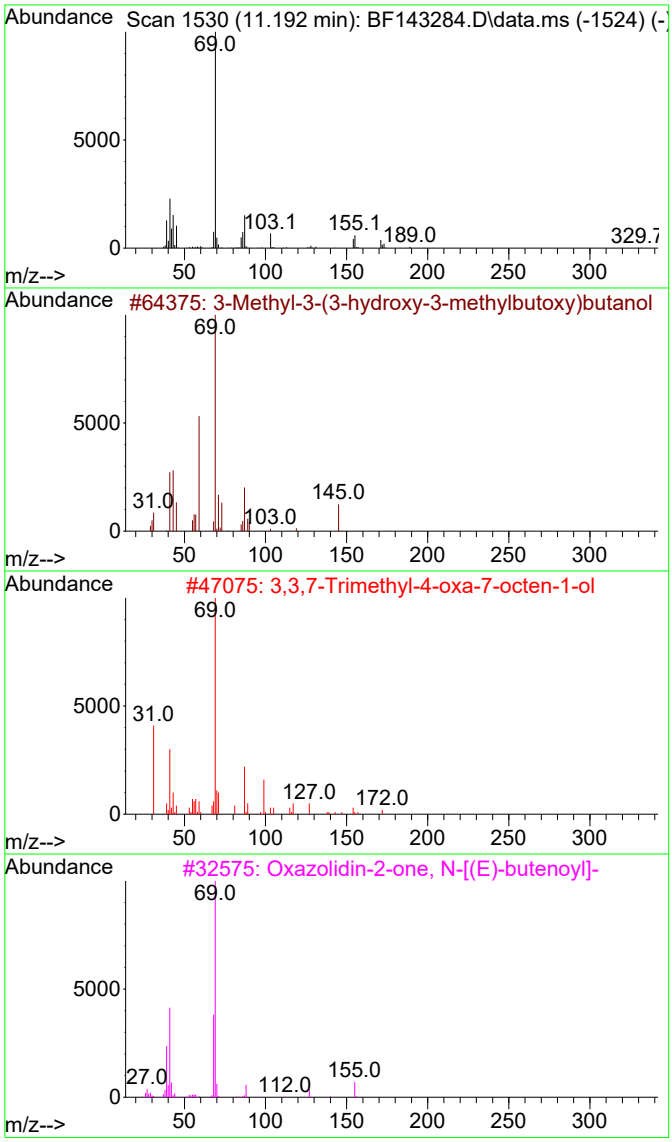
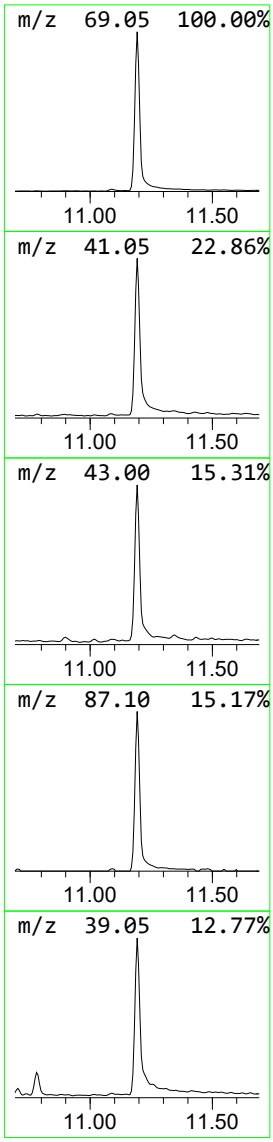
Peak Number 11 unknown11.192 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.192	10.62 ng	414915	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-3-(3-hydroxy-3-methylbu...	190	C10H22O3	1000432-16-8	39
2	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	38
3	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1010156-45-5	33
4	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
5	Cyclopropanecarboxylic acid chlo...	104	C4H5ClO	004023-34-1	9





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Data File : BF143284.D
Acq On : 01 Aug 2025 16:03
Operator : RC/JU
Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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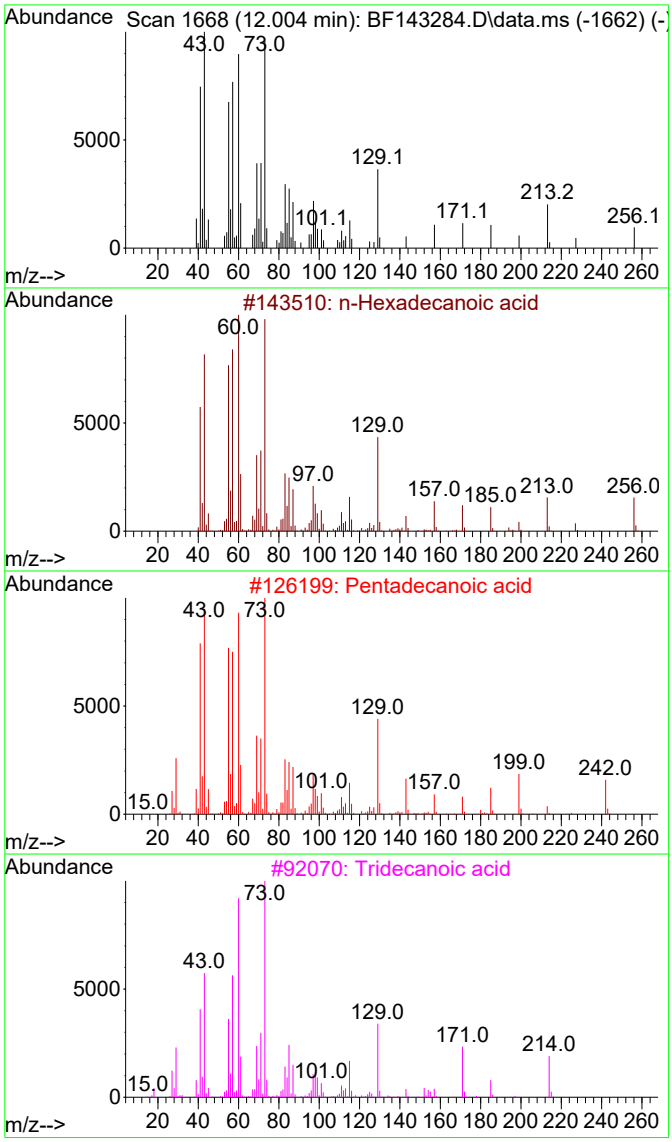
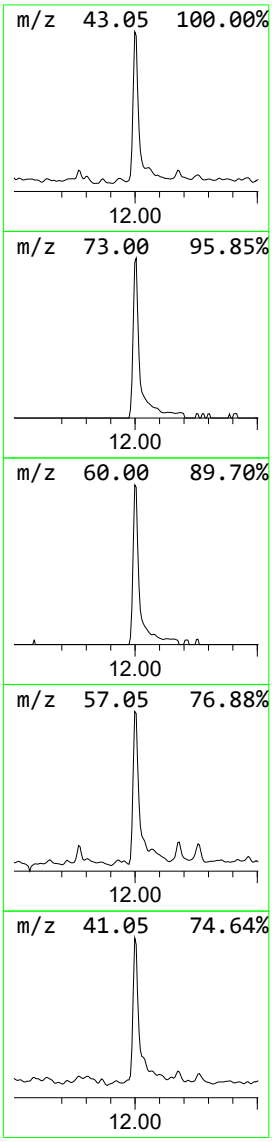
Peak Number 12 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	3.31 ng	129124	Phenanthrene-d10	11.480

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	18





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Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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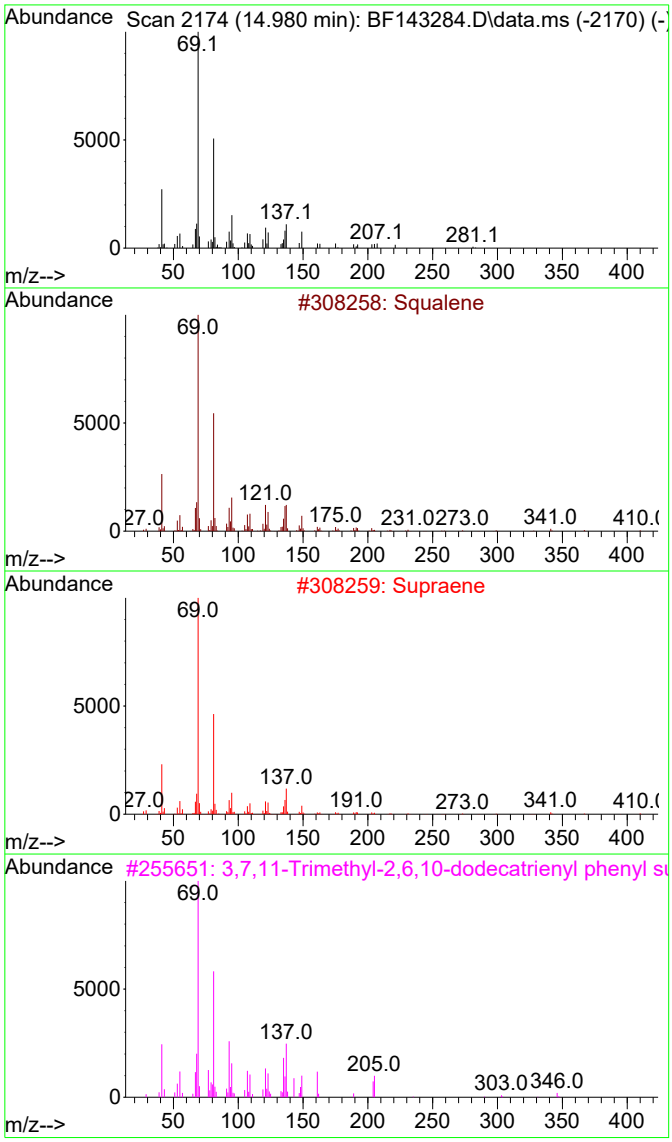
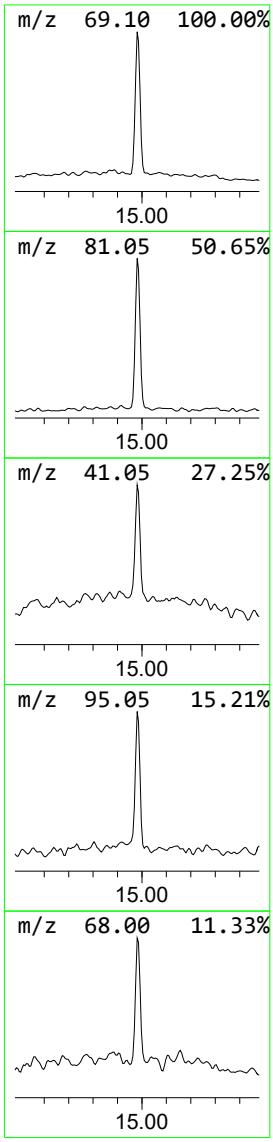
Peak Number 13 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	2.32 ng	63173	Perylene-d12	15.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	90
3	3,7,11-Trimethyl-2,6,10-dodecatr...	346	C21H30O2S	1000432-39-0	78
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080125\
Data File : BF143284.D
Acq On : 01 Aug 2025 16:03
Operator : RC/JU
Sample : Q2733-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.310	92.2	ng	3425340	1	6.957	742701	20.0
Propanoic acid,...	4.110	9.9	ng	368341	1	6.957	742701	20.0
Butanoic acid	4.687	24.3	ng	900987	1	6.957	742701	20.0
2-Pentanone, 4-...	5.193	7.3	ng	269703	1	6.957	742701	20.0
Butanoic acid, ...	5.369	16.7	ng	619918	1	6.957	742701	20.0
Butanoic acid, ...	5.522	11.9	ng	440017	1	6.957	742701	20.0
Pentanoic acid	5.757	4.7	ng	175030	1	6.957	742701	20.0
Ethanol, 2-butoxy-	5.934	2.0	ng	76220	1	6.957	742701	20.0
Cyclopropanecar...	8.934	15.6	ng	695325	2	8.239	892442	20.0
Benzophenone	10.704	3.1	ng	151798	3	9.992	975692	20.0
unknown11.192	11.192	10.6	ng	414915	4	11.480	781373	20.0
n-Hexadecanoic ...	12.004	3.3	ng	129124	4	11.480	781373	20.0
Squalene	14.980	2.3	ng	63173	6	15.627	543503	20.0