LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-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_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028475.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.663	68	81	85	rBV2	21485	52023	5.02%	0.685%
2	3.999	131	138	143	rVB	10864	17625	1.70%	0.232%
3	4.828	271	279	286	rBV	13660	24616	2.38%	0.324%
4	4.975	295	304	309	rBV	9334	16419	1.59%	0.216%
5	5.075	316	321	329	rVB	29941	41319	3.99%	0.544%
6	5.440	378	383	393	rVB	7294	12115	1.17%	0.159%
7	5.552	396	402	412	rVB	438327	651669	62.92%	8.577%
8	6.416	538	549	553	rBV	20184	43538	4.20%	0.573%
9	7.187	673	680	693	rVB	422418	686653	66.29%	9.038%
10	7.963	804	812	817	rBV	15115	26673	2.58%	0.351%
11	8.034	817	824	831	rVB	138284	218633	21.11%	2.878%
12	9.204	1014	1023	1035	rBV	272587	436812	42.17%	5.749%
13	10.081	1165	1172	1179	rBV	8769	16608	1.60%	0.219%
14	10.845	1295	1302	1310	rVB	174957	293381	28.33%	3.861%
15	13.298	1712	1719	1726	rBV	595894	857315	82.77%	11.284%
16	14.122	1854	1859	1865	rVB	26922	34569	3.34%	0.455%
17	14.504	1916	1924	1929	rBV2	5579	12613	1.22%	0.166%
18	14.669	1947	1952	1960	rVB2	236691	349883	33.78%	4.605%
19	16.151	2196	2204	2210	rBV	458018	630368	60.86%	8.297%
20	17.280	2392	2396	2399	rBV2	9712	12548	1.21%	0.165%
21	17.398	2410	2416	2424	rBV	271196	385345	37.20%	5.072%
22	17.762	2471	2478	2483	rBV4	7118	11958	1.15%	0.157%
23	18.157	2538	2545	2550	rBV3	6369	11632	1.12%	0.153%
24	18.274	2559	2565	2576	rBV	118481	179848	17.36%	2.367%
25	18.562	2610	2614	2622	rBV6	6054	12760	1.23%	0.168%
26	19.421	2753	2760	2762	rBV6	12436	23924	2.31%	0.315%
27	19.533	2775	2779	2785	rBV	23921	33497	3.23%	0.441%
28	19.986	2851	2856	2861	rBV	823314	1035757	100.00%	13.632%
29	21.074	3037	3041	3047	rBV	134675	149391	14.42%	1.966%
30	21.221	3062	3066	3071	rBV	158916	197225	19.04%	2.596%
31	21.527	3113	3118	3125	rBV	337624	422641	40.81%	5.563%
32	22.115	3216	3218	3224	rVB2	46847	55891	5.40%	0.736%
33	23.086	3379	3383	3388	rVB	65961	91440	8.83%	1.204%
34	23.815	3501	3507	3514	rVB2	213400	417196	40.28%	5.491%
35	24.333	3591	3595	3601	rVB	72675	133886	12.93%	1.762%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BASIN-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_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

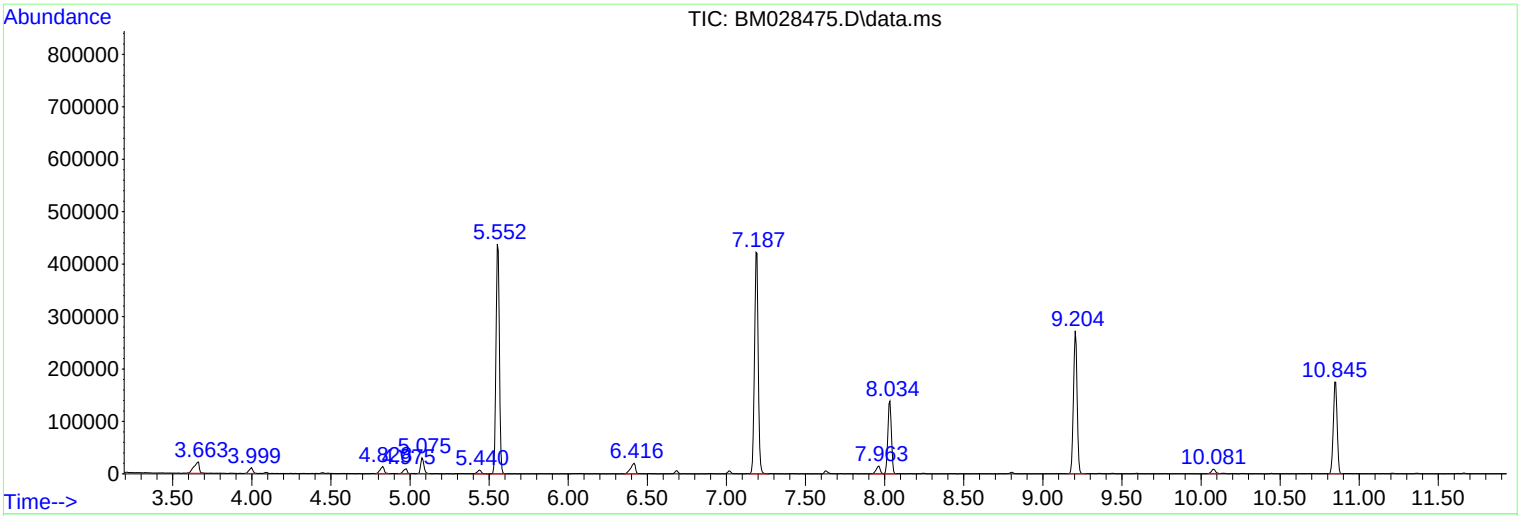
Sum of corrected areas: 7597771

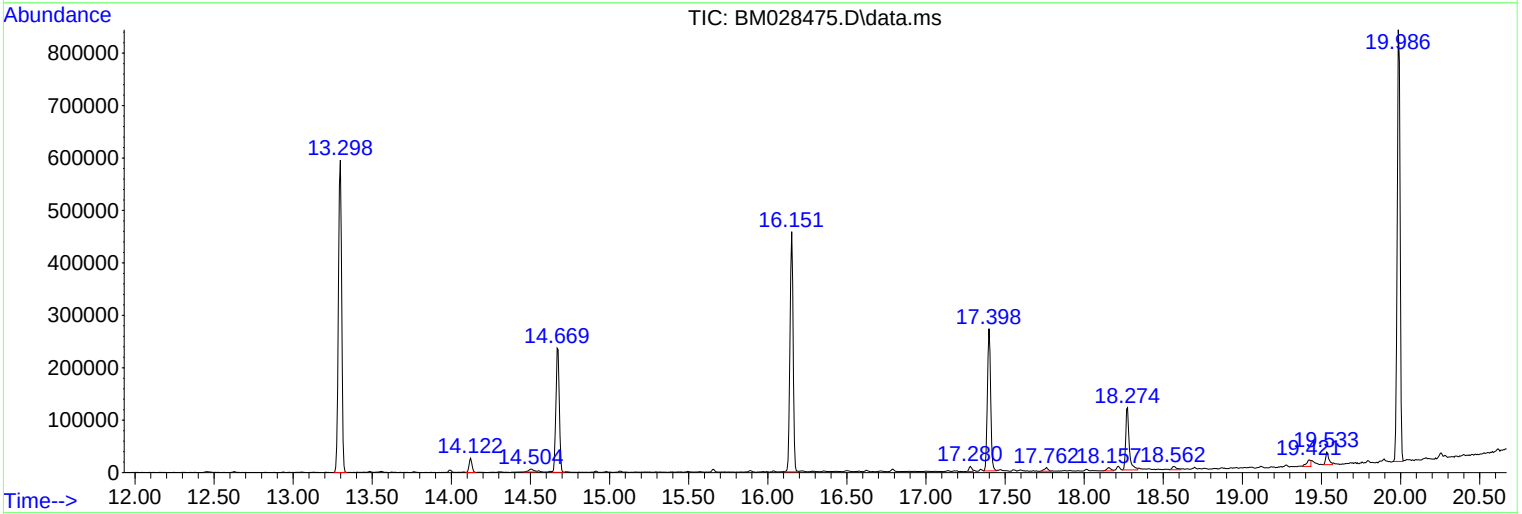
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

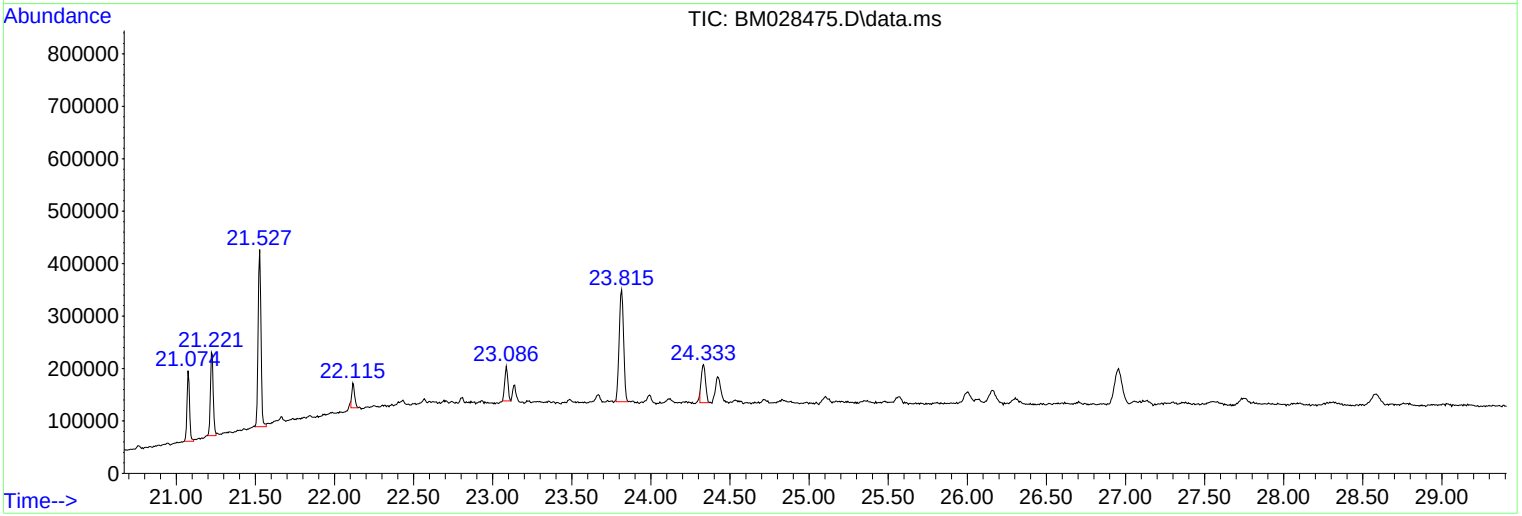
Instrument :
BNA_M
ClientSampleId :
BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

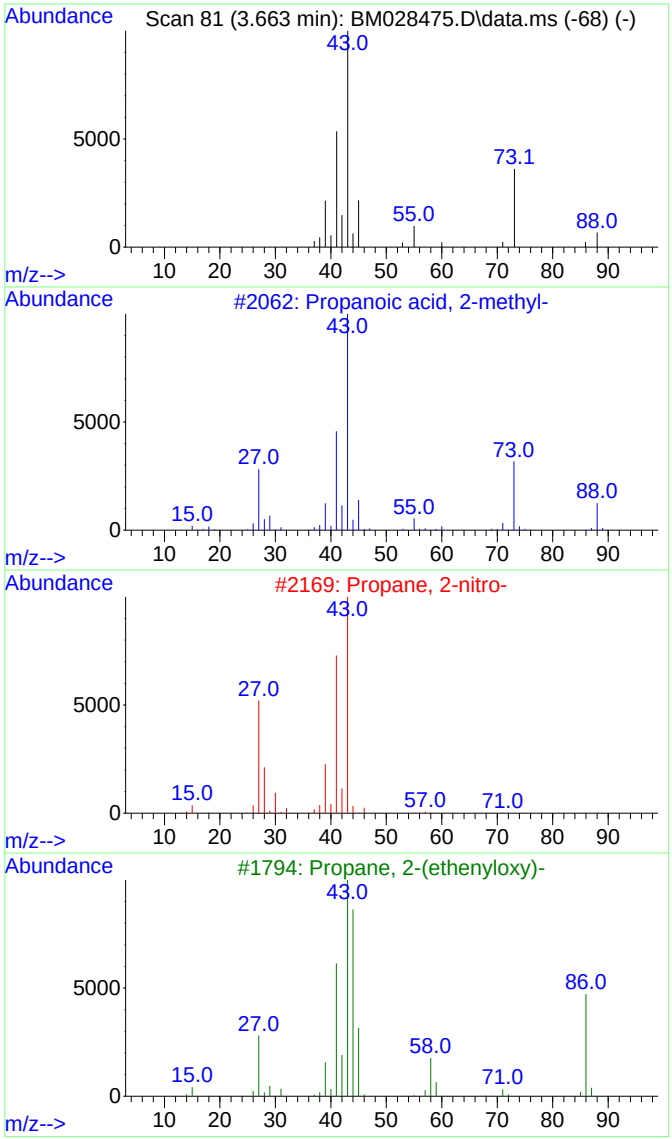
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

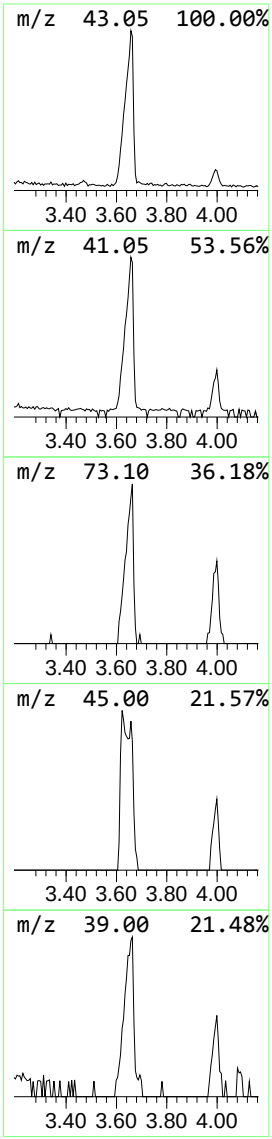
****

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.663	4.76 ng	52023	1,4-Dichlorobenzene-d4	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	86
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	17
3	Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	9
4	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	9
5	1-Propanesulfonyl chloride	142	C3H7ClO2S	010147-36-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

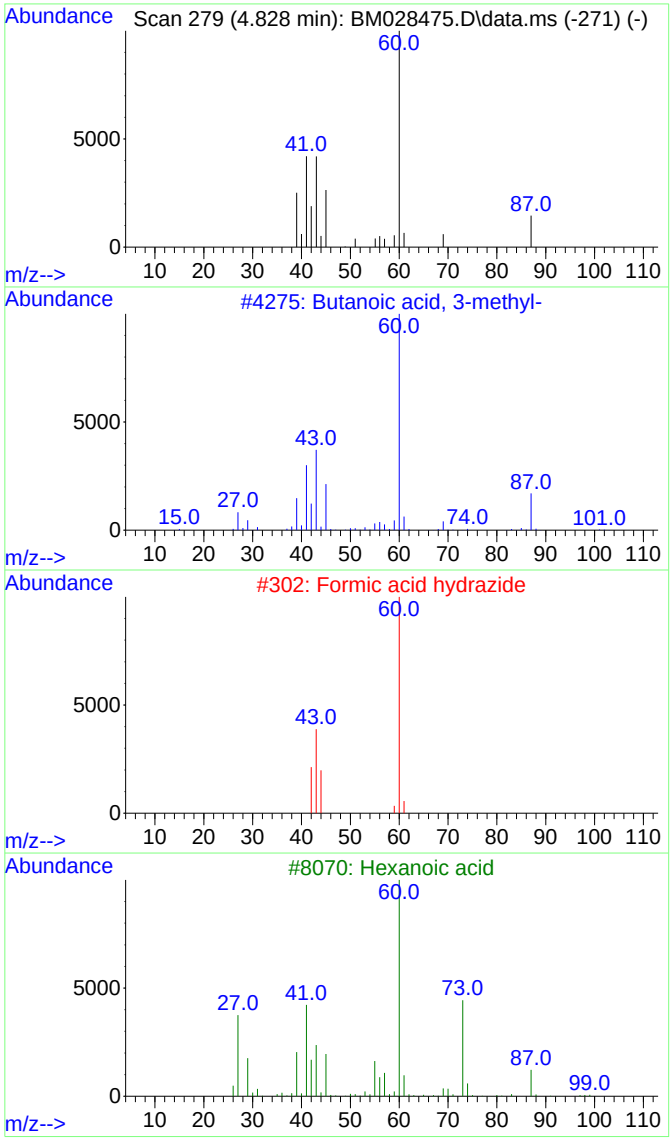
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

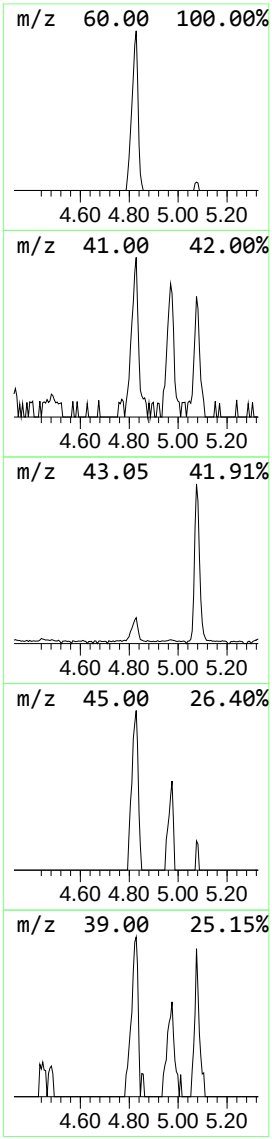
****

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.828	2.25 ng	24616	1,4-Dichlorobenzene-d4	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	40
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	1-Hexanamine	101	C6H15N	000111-26-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BASIN-1

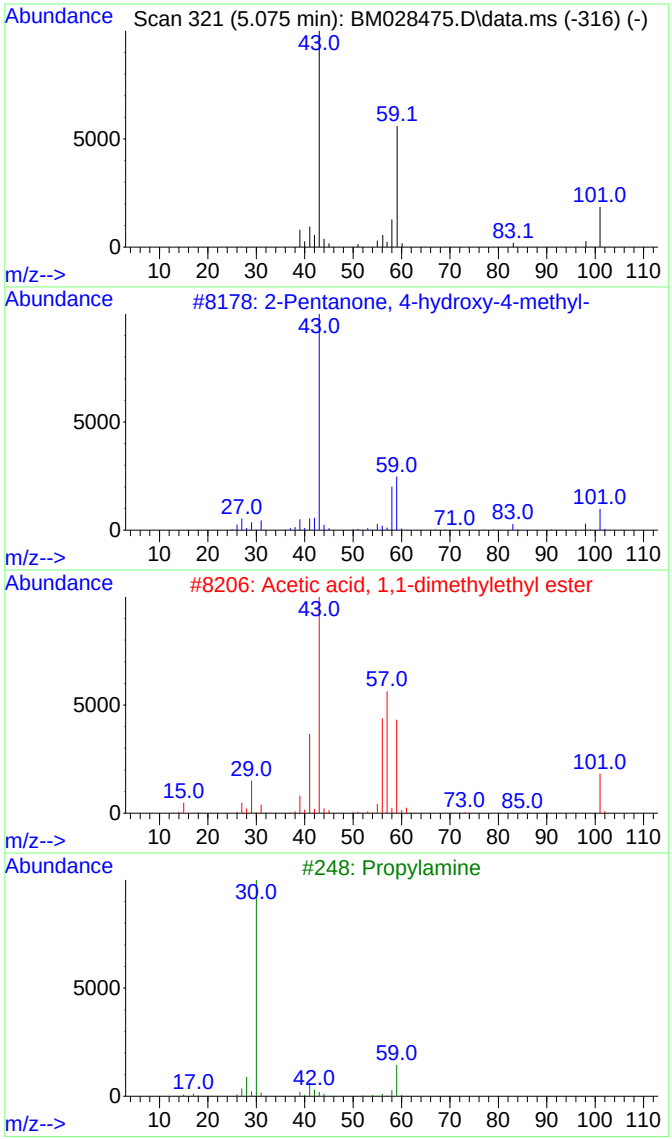
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

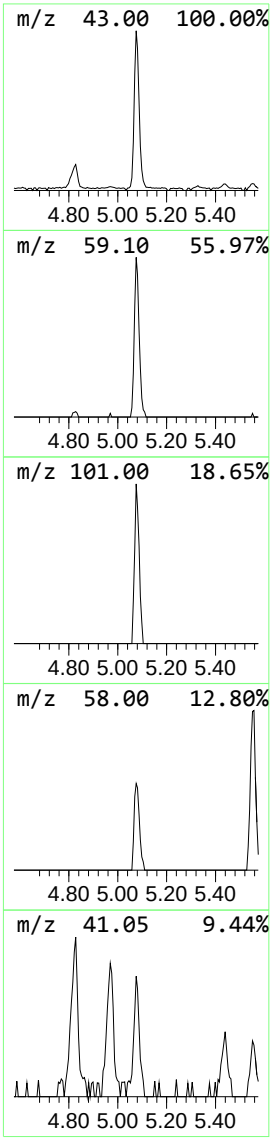
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.78 ng	41319	1,4-Dichlorobenzene-d4	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propylamine	59	C3H9N	000107-10-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

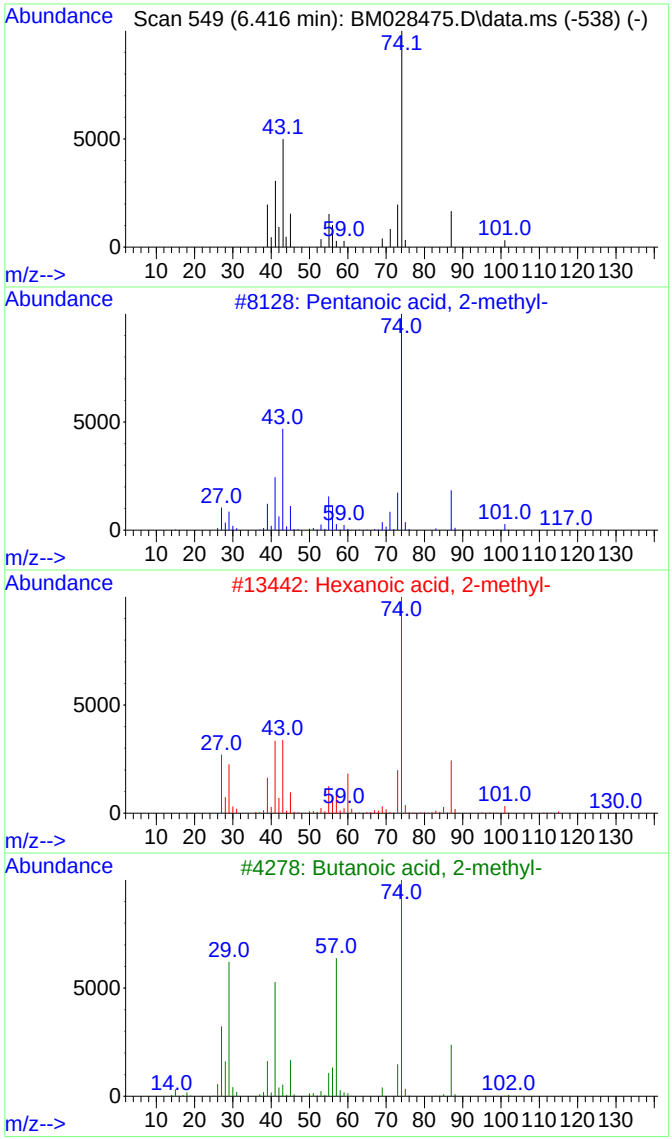
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

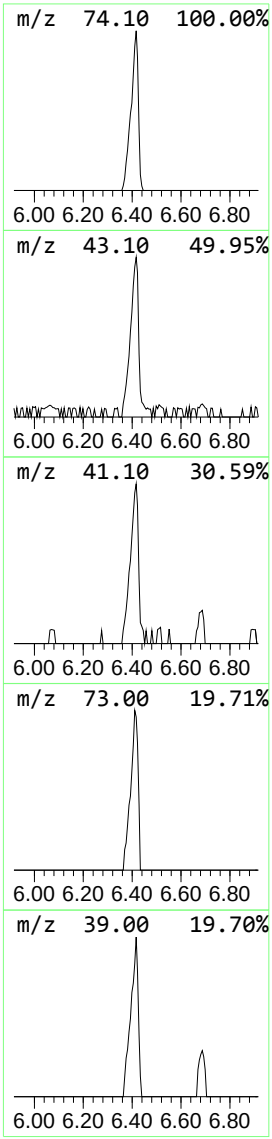
****

Peak Number 4 Pentanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.416	3.98 ng	43538	1,4-Dichlorobenzene-d4	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	64
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	39
4	Diethanolamine	105	C4H11NO2	000111-42-2	33
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

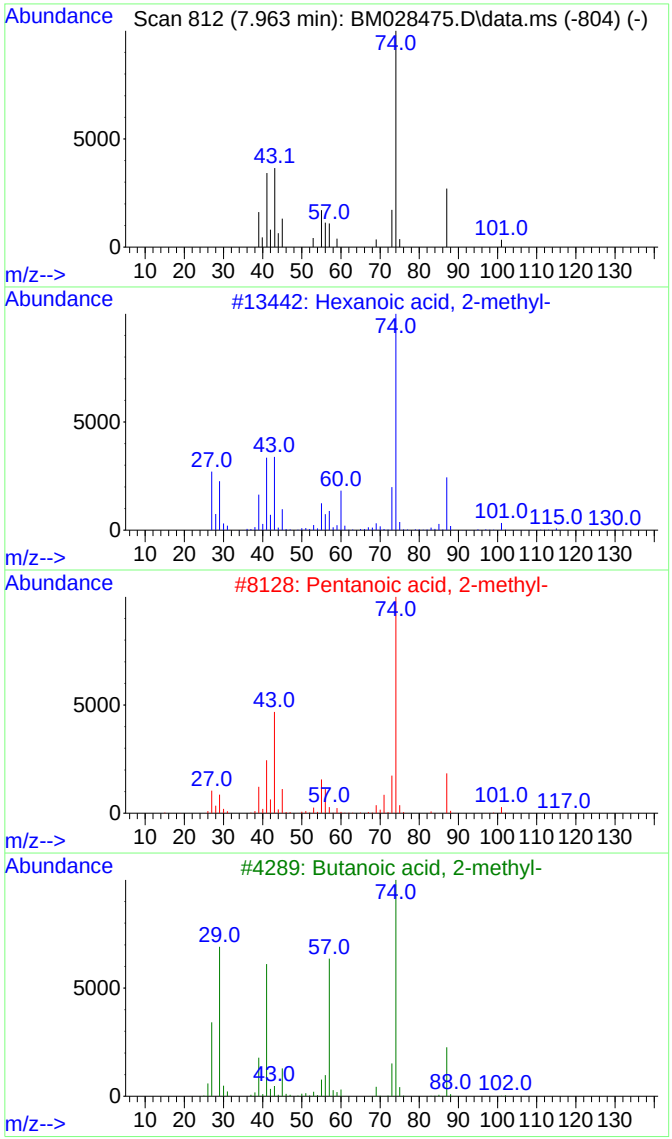
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

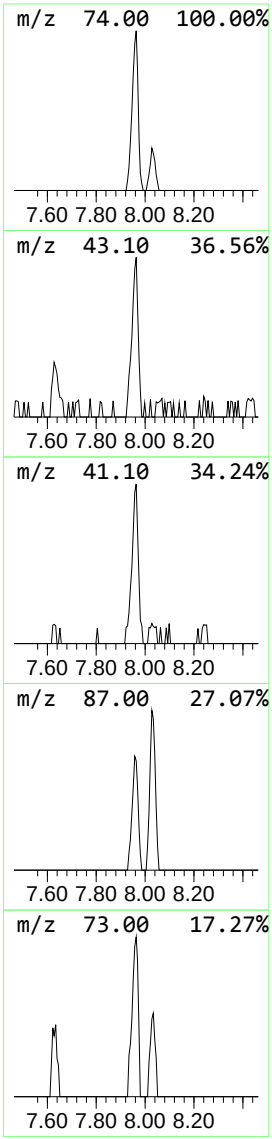
****

Peak Number 5 Hexanoic acid, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.963	2.44 ng	26673	1,4-Dichlorobenzene-d4	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	83
2	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	72
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
4	2-Methylheptanoic acid	144	C8H16O2	001188-02-9	39
5	Methyl valerate	116	C6H12O2	000624-24-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

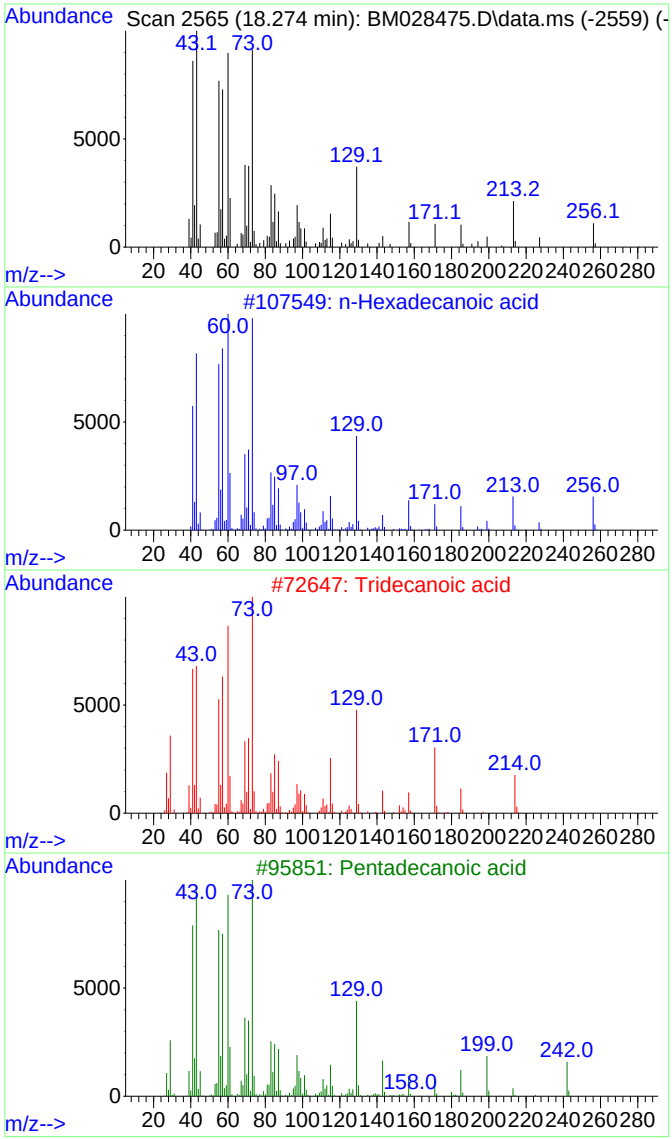
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

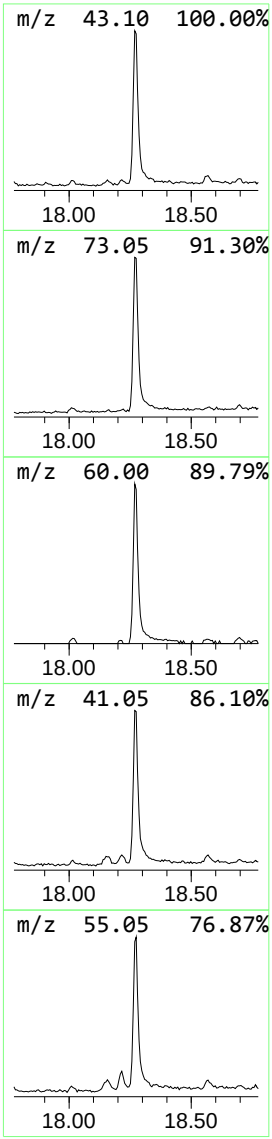
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	9.33 ng	179848	Phenanthrene-d10	17.398

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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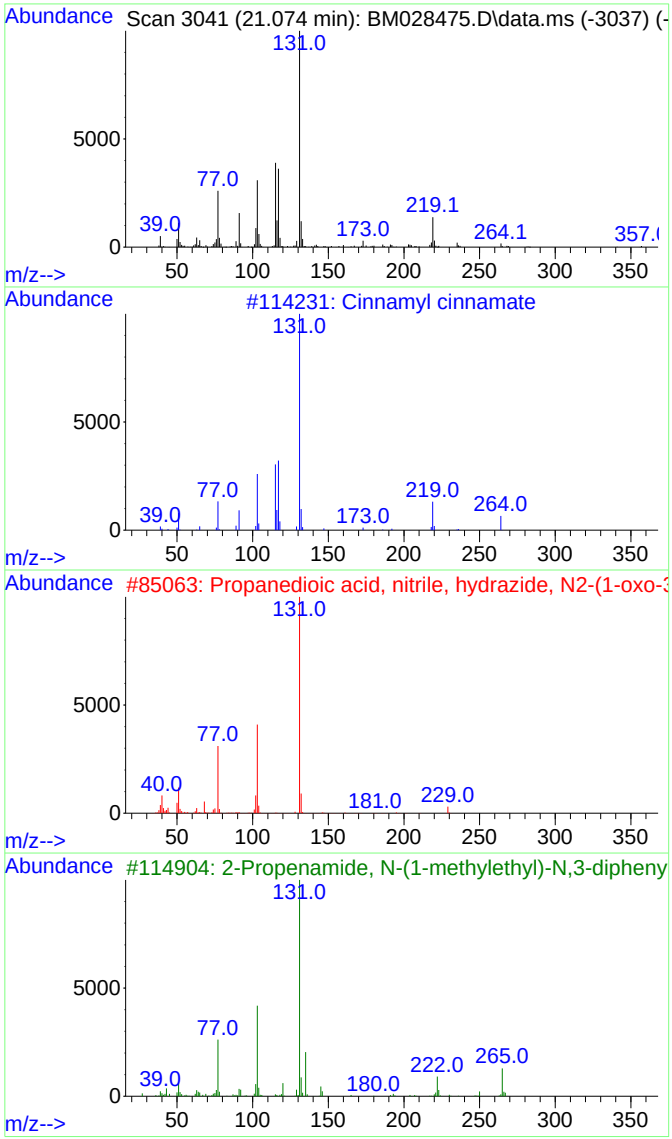
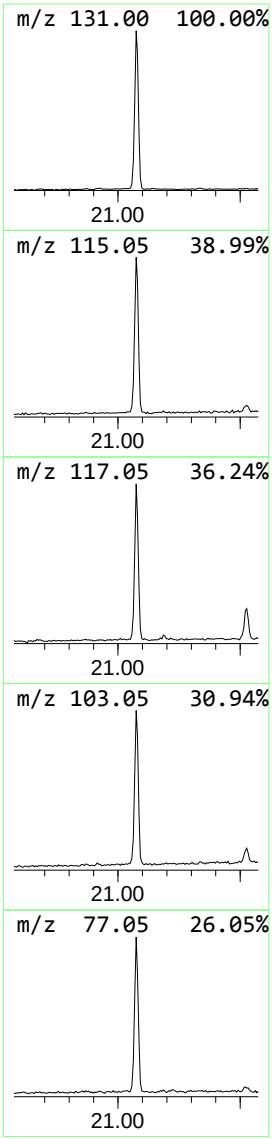
Peak Number 7 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	7.07 ng	149391	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	86
2	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	49
3	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	47
4	2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	47
5	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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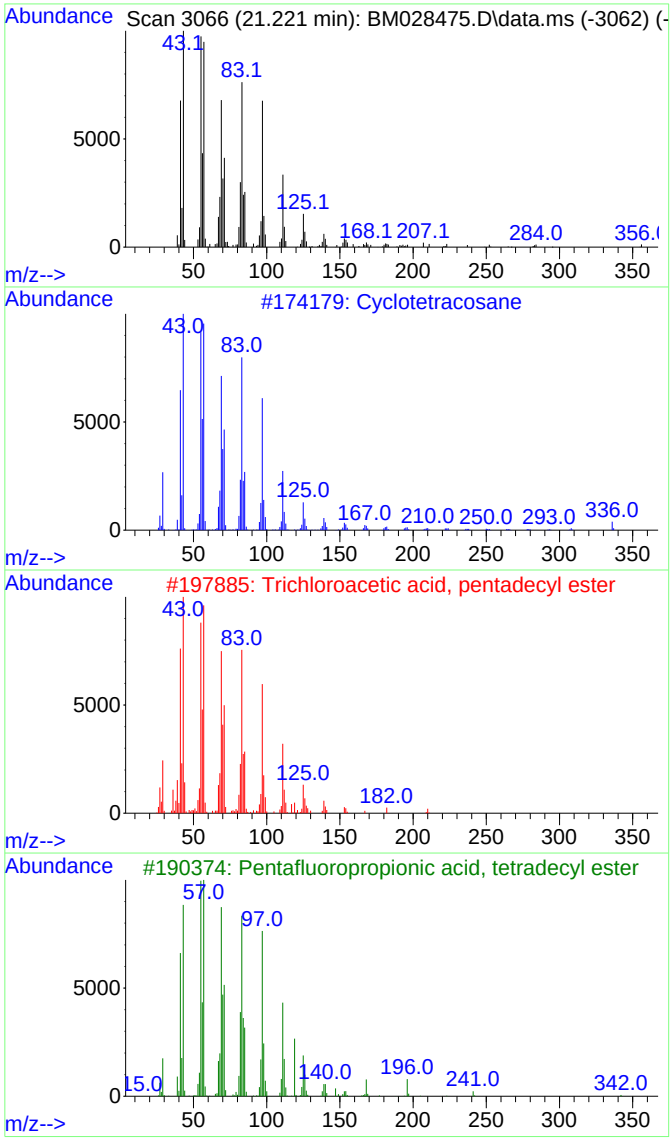
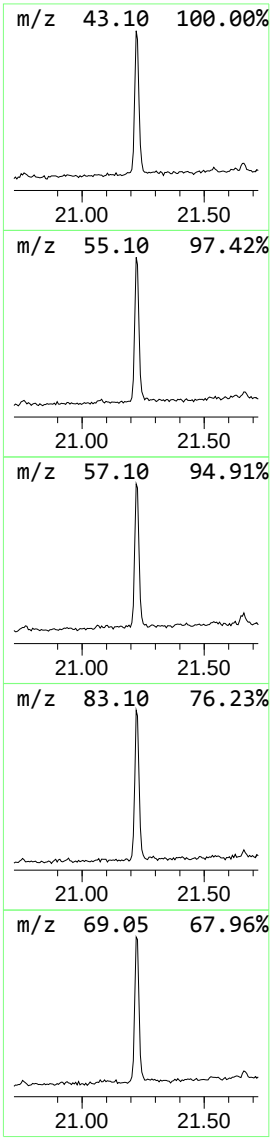
Peak Number 8 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	9.33 ng	197225	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
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Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Integration Parameters: LSCINT.P

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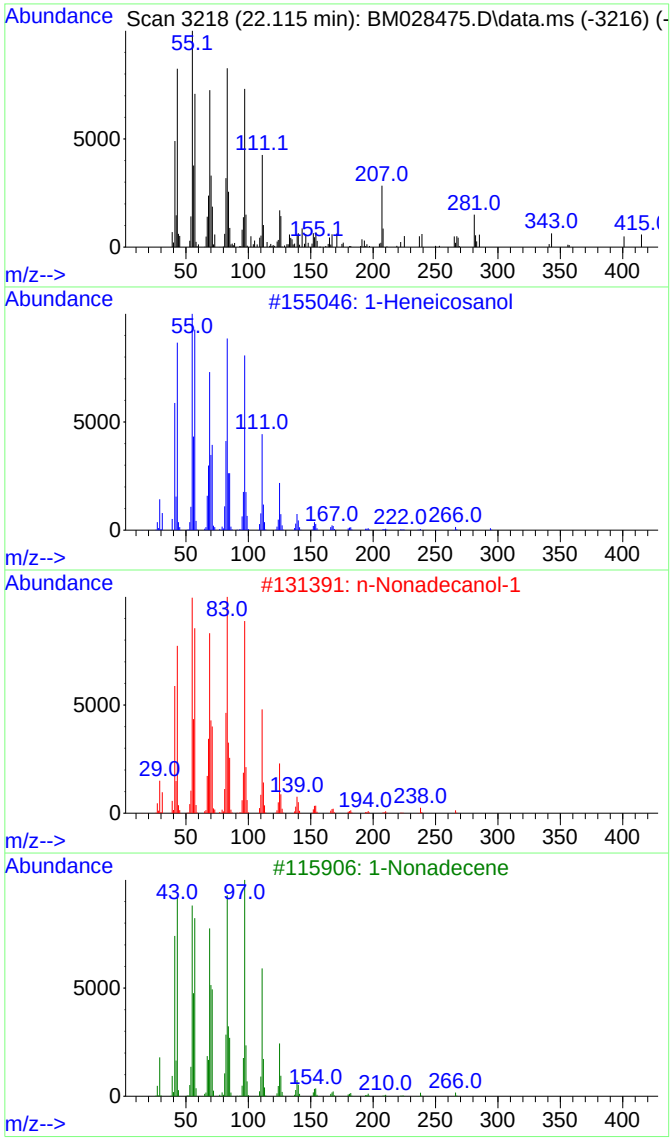
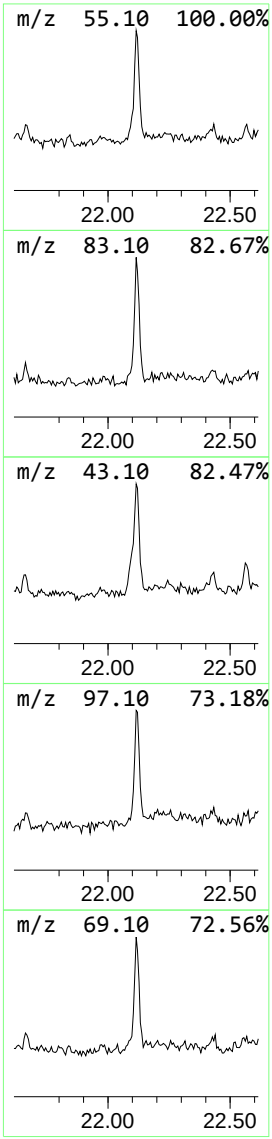
Peak Number 9 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.115	2.64 ng	55891	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	90
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	1-Nonadecene	266	C19H38	018435-45-5	83
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74





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Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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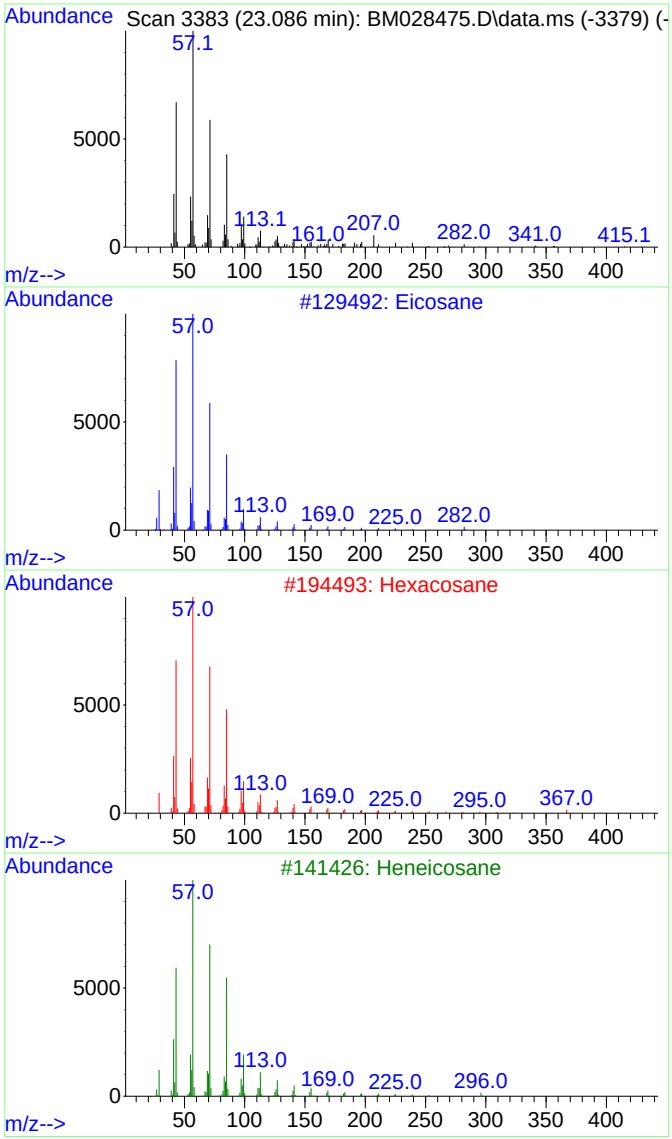
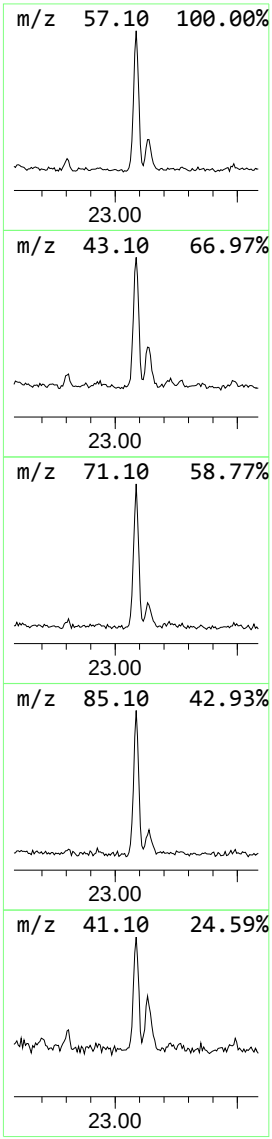
Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	4.38 ng	91440	Perylene-d12	23.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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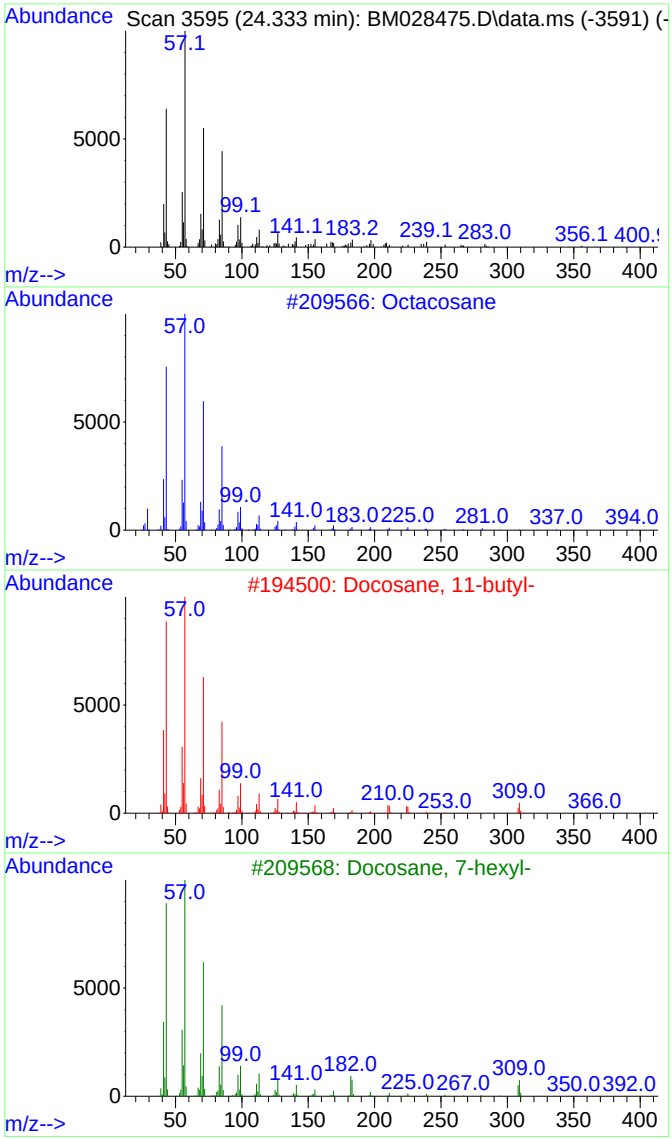
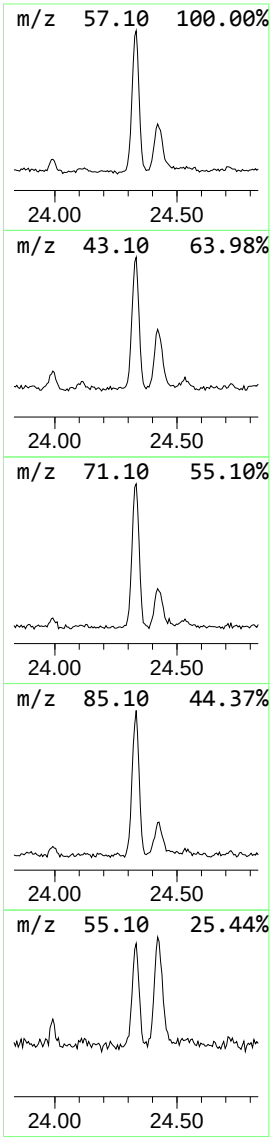
Peak Number 11 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.333	6.42 ng	133886	Perylene-d12	23.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028475.D
Acq On : 20 Jan 2021 19:31
Operator : CG/JU
Sample : M1160-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BASIN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid,...	3.663	4.8	ng	52023	1	8.034	218633	20.0
Butanoic acid, ...	4.828	2.3	ng	24616	1	8.034	218633	20.0
2-Pentanone, 4-...	5.075	3.8	ng	41319	1	8.034	218633	20.0
Pentanoic acid,...	6.416	4.0	ng	43538	1	8.034	218633	20.0
Hexanoic acid, ...	7.963	2.4	ng	26673	1	8.034	218633	20.0
n-Hexadecanoic ...	18.274	9.3	ng	179848	4	17.398	385345	20.0
Cinnamyl cinnamate	21.074	7.1	ng	149391	5	21.527	422641	20.0
Cyclotetracosane	21.221	9.3	ng	197225	5	21.527	422641	20.0
1-Heneicosanol	22.115	2.6	ng	55891	5	21.527	422641	20.0
Eicosane	23.086	4.4	ng	91440	6	23.815	417196	20.0
Octacosane	24.333	6.4	ng	133886	6	23.815	417196	20.0