LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

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-BM121620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.722	88	91	99	rBV	20795	33912	1.26%	0.098%
2	5.216	338	345	352	rVB	20275	33124	1.23%	0.095%
3	5.693	419	426	436	rBV	1675956	2419243	89.92%	6.969%
4	6.846	615	622	629	rVB	38269	60467	2.25%	0.174%
5	7.157	667	675	682	rBV3	18450	32066	1.19%	0.092%
6	7.334	697	705	719	rBV	1528221	2510598	93.31%	7.232%
7	7.775	775	780	793	rBV	90416	148924	5.54%	0.429%
8	8.193	844	851	858	rBV	501365	794742	29.54%	2.289%
9	9.369	1043	1051	1059	rBV	959795	1581822	58.79%	4.557%
10	11.022	1324	1332	1340	rVB	637080	1036151	38.51%	2.985%
11	13.451	1735	1745	1752	rBV	1825905	2660010	98.87%	7.663%
12	13.704	1781	1788	1796	rBV	675716	1038604	38.60%	2.992%
13	14.151	1858	1864	1869	rBV5	24400	38321	1.42%	0.110%
14	14.263	1876	1883	1892	rBV	147830	243198	9.04%	0.701%
15	14.545	1924	1931	1932	rBV4	15246	28070	1.04%	0.081%
16	14.651	1945	1949	1954	rVB5	30312	47894	1.78%	0.138%
17	14.780	1966	1971	1973	rBV5	31405	55984	2.08%	0.161%
18	14.822	1973	1978	1984	rVV	813739	1210158	44.98%	3.486%
19	14.886	1985	1989	1994	rVV2	22778	36462	1.36%	0.105%
20	15.210	2039	2044	2048	rBV5	19464	35152	1.31%	0.101%
21	15.433	2078	2082	2085	rBV6	17726	30802	1.14%	0.089%
22	15.598	2105	2110	2114	rBV3	38222	65482	2.43%	0.189%
23	15.857	2149	2154	2158	rBV3	38809	66678	2.48%	0.192%
24	15.910	2159	2163	2171	rVV	150257	221256	8.22%	0.637%
25	16.298	2223	2229	2239	rBV	1402451	2026232	75.31%	5.837%
26	16.516	2262	2266	2271	rVB	95735	127890	4.75%	0.368%
27	17.327	2401	2404	2408	rVB	89912	109911	4.09%	0.317%
28	17.545	2435	2441	2445	rBV	906034	1332118	49.51%	3.837%
29	17.586	2445	2448	2454	rVB	468196	629085	23.38%	1.812%
30	17.674	2460	2463	2467	rVB	70737	91789	3.41%	0.264%
31	17.933	2504	2507	2512	rVB2	79177	106420	3.96%	0.307%
32	18.398	2582	2586	2592	rBV3	197525	314341	11.68%	0.906%
33	19.568	2780	2785	2791	rVB	983029	1305629	48.53%	3.761%
34	19.657	2797	2800	2804	rVB2	63795	82326	3.06%	0.237%
35	19.898	2836	2841	2842	rBV2	126400	188693	7.01%	0.544%
36	19.927	2842	2846	2854	rVB	757962	999553	37.15%	2.879%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

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-BM121620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.115	2873	2878	2883	rVB	2158031	2690490	100.00%	7.750%
38	20.409	2925	2928	2933	rVB2	123063	172699	6.42%	0.497%
39	20.509	2942	2945	2949	rVB	73170	82413	3.06%	0.237%
40	21.345	3084	3087	3092	rBV	450154	568802	21.14%	1.639%
41	21.656	3134	3140	3144	rBV2	1250903	2118562	78.74%	6.103%
42	21.698	3144	3147	3152	rVB	398874	497120	18.48%	1.432%
43	21.974	3191	3194	3200	rVB2	140400	189506	7.04%	0.546%
44	22.233	3235	3238	3240	rBV2	252921	300939	11.19%	0.867%
45	22.262	3240	3243	3254	rVB3	354850	600871	22.33%	1.731%
46	22.968	3360	3363	3369	rVB	206731	277132	10.30%	0.798%
47	23.262	3408	3413	3417	rBV	734990	1168845	43.44%	3.367%
48	23.309	3417	3421	3433	rVB	449974	1270757	47.23%	3.661%
49	23.921	3521	3525	3532	rVB	264540	497253	18.48%	1.432%
50	24.027	3537	3543	3549	rVV	687920	1227140	45.61%	3.535%
51	24.203	3570	3573	3578	rVB	209293	301548	11.21%	0.869%
52	24.556	3628	3633	3642	rVB	501105	1006800	37.42%	2.900%

Sum of corrected areas: 34713984

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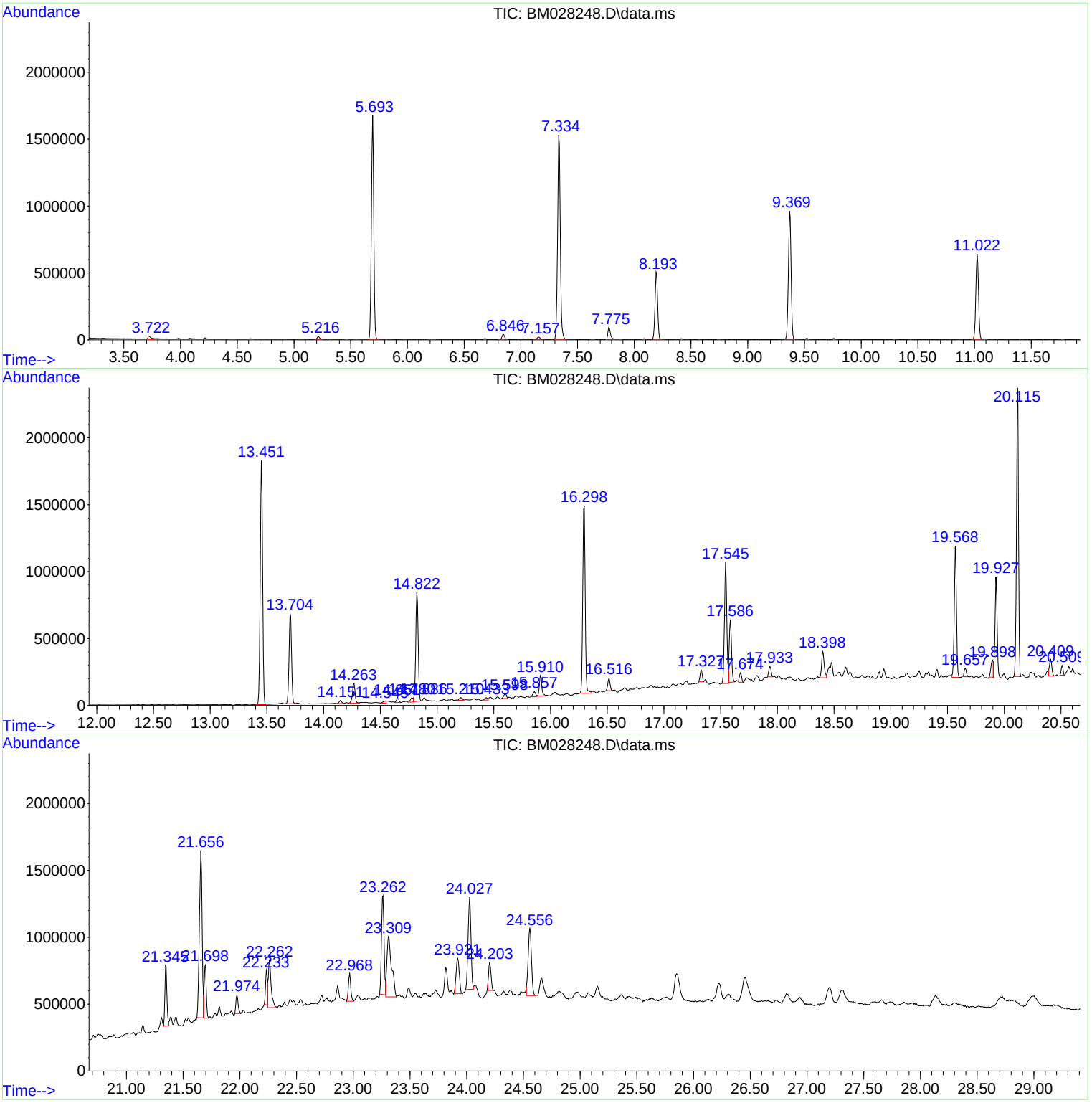
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

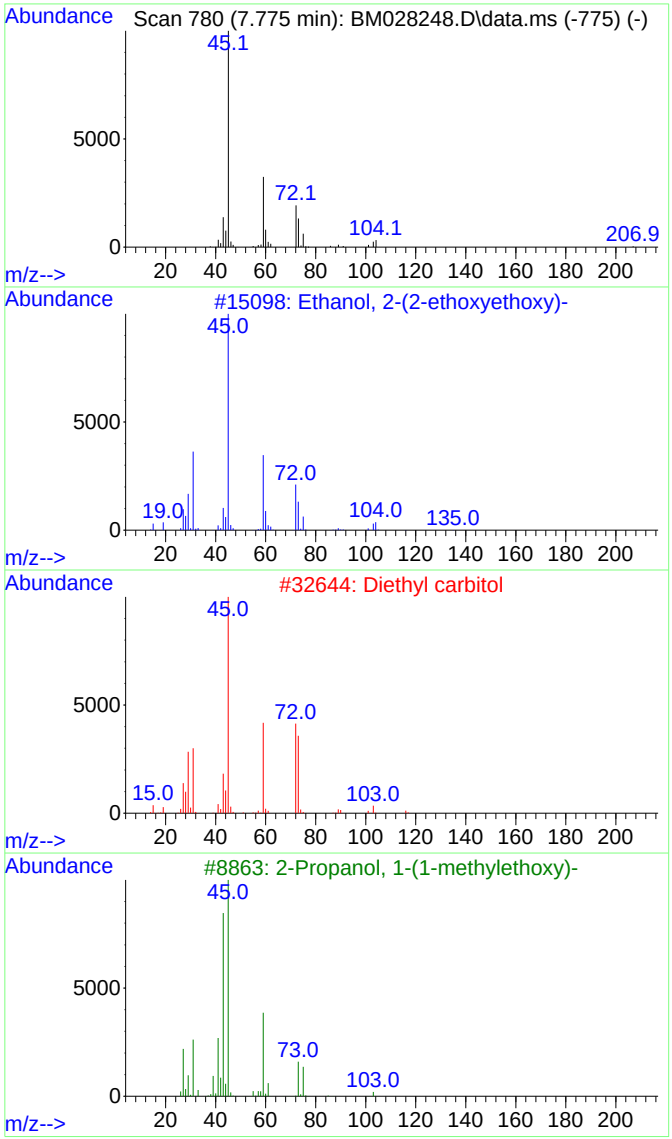
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

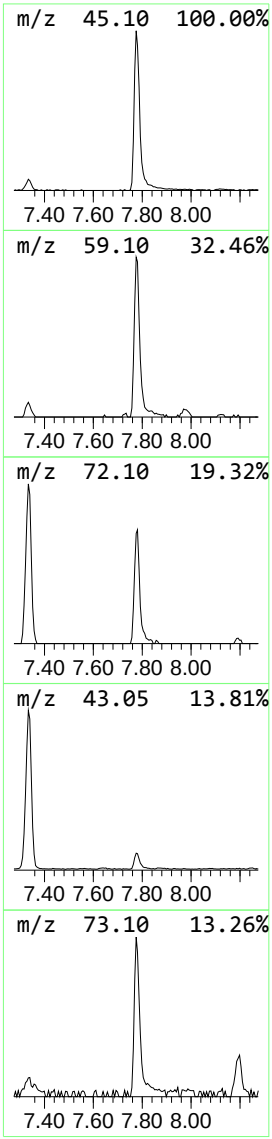
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.775	3.75 ng	148924	1,4-Dichlorobenzene-d4	8.193

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	78
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	36
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

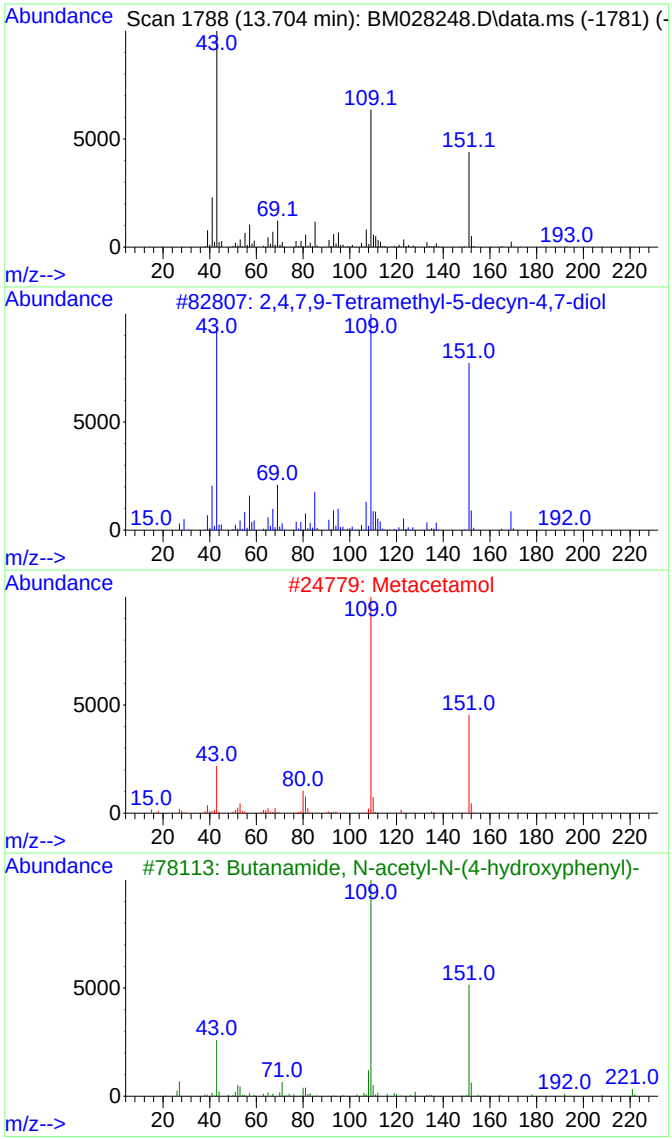
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

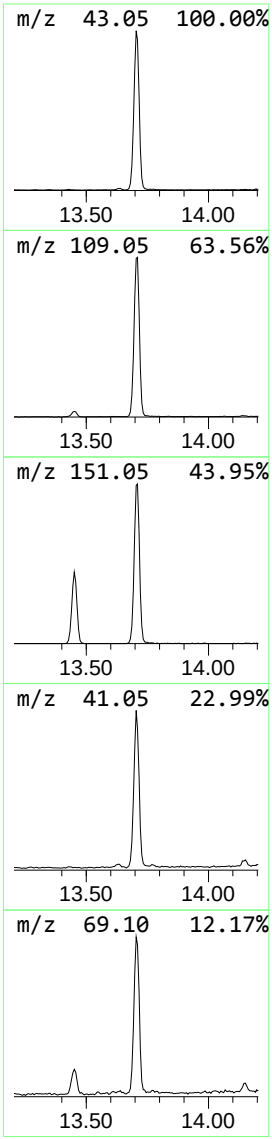
****

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.704	17.16 ng	1038600	Acenaphthene-d10	14.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Metacetamol	151	C8H9NO2	000621-42-1	53
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	42
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

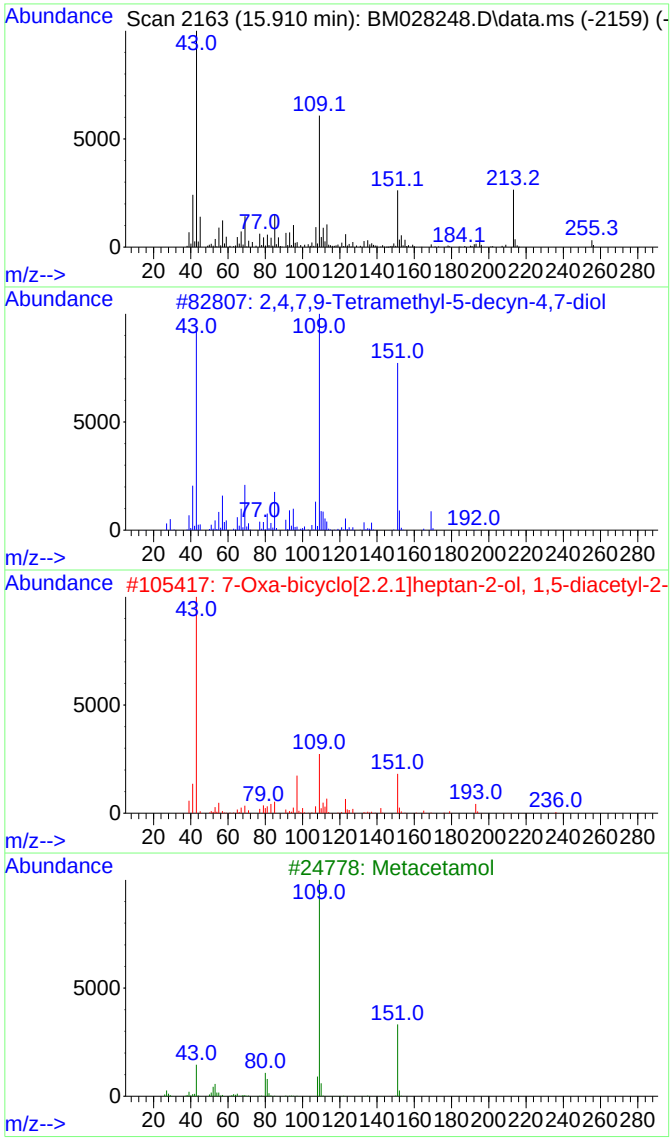
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

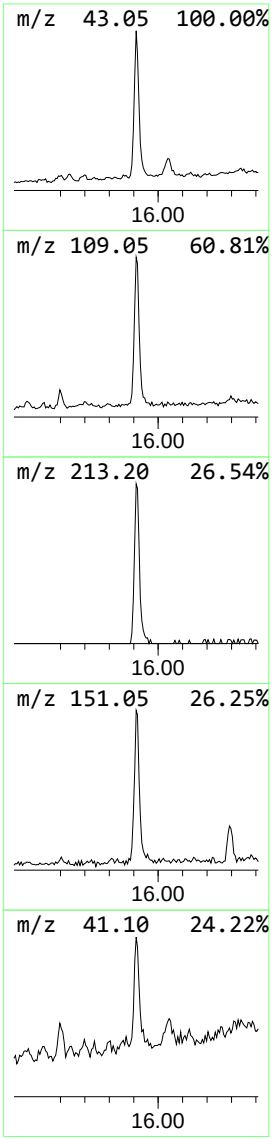
****

Peak Number 3 unknown15.91 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	3.66 ng	221256	Acenaphthene-d10	14.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58
2	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	42
3	Metacetamol	151	C8H9NO2	000621-42-1	38
4	Acetaminophen	151	C8H9NO2	000103-90-2	38
5	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

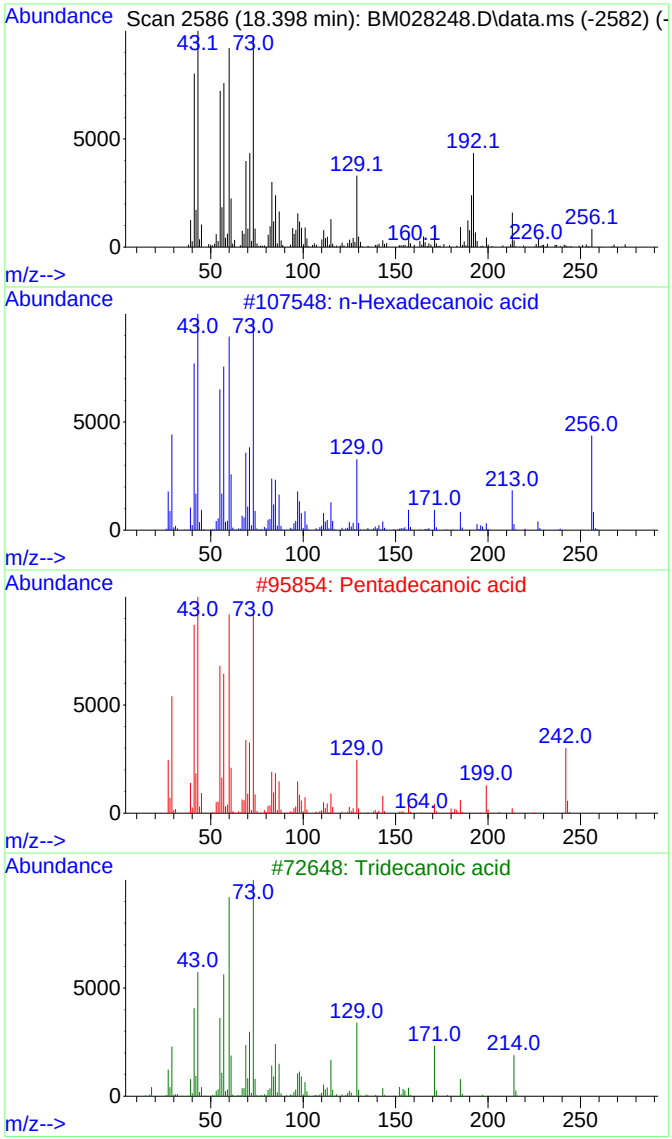
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

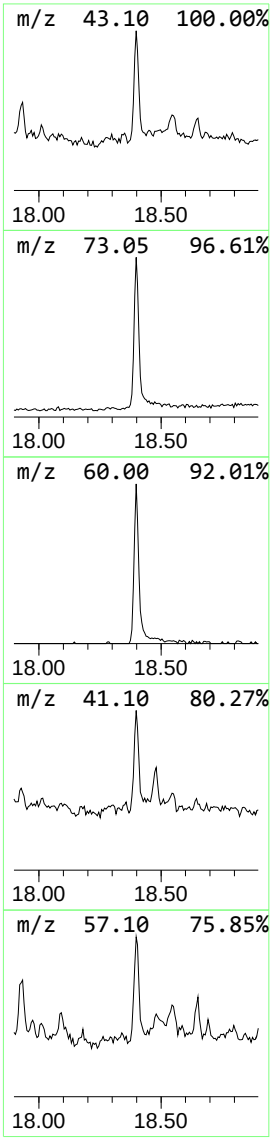
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	4.72 ng	314341	Phenanthrene-d10	17.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

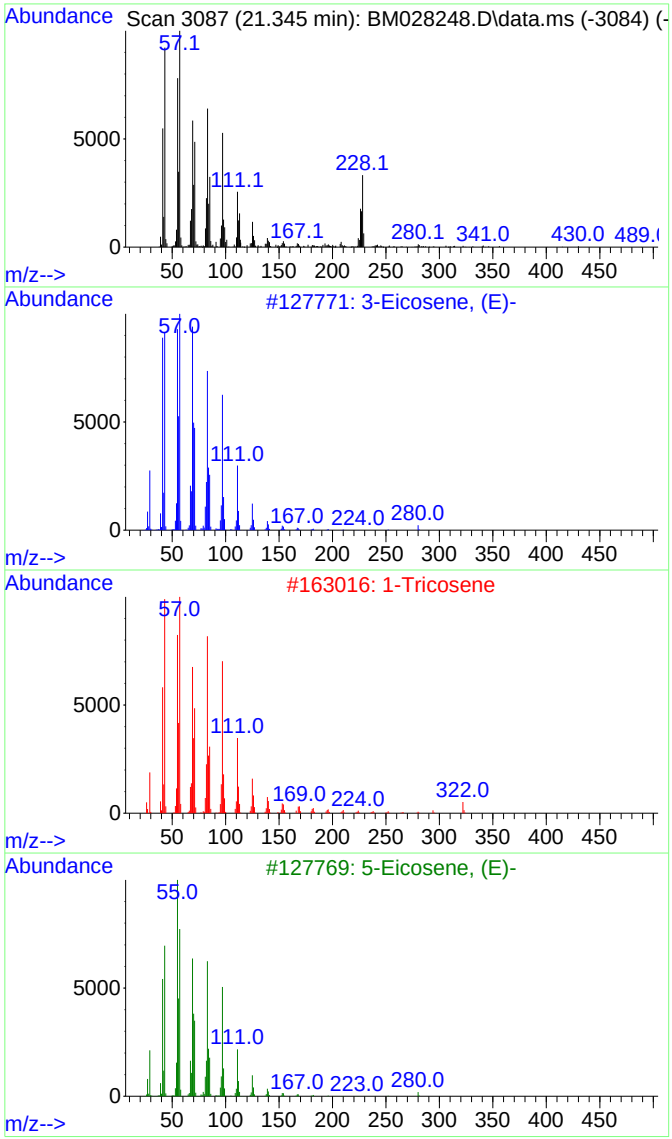
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

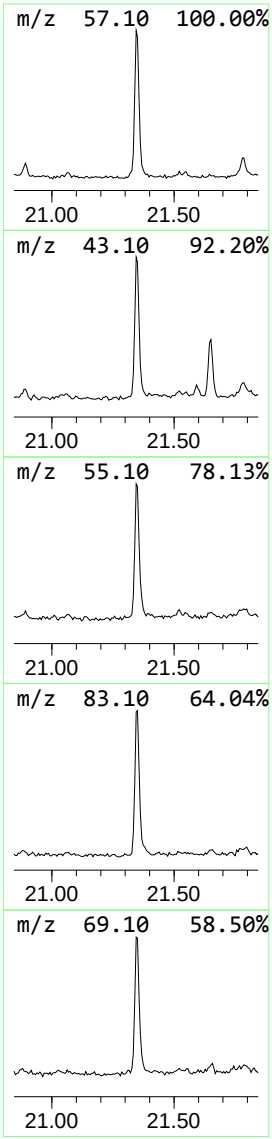
****

Peak Number 5 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.345	5.37 ng	568802	Chrysene-d12	21.656

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	1-Tricosene	322	C23H46	018835-32-0	96
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
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Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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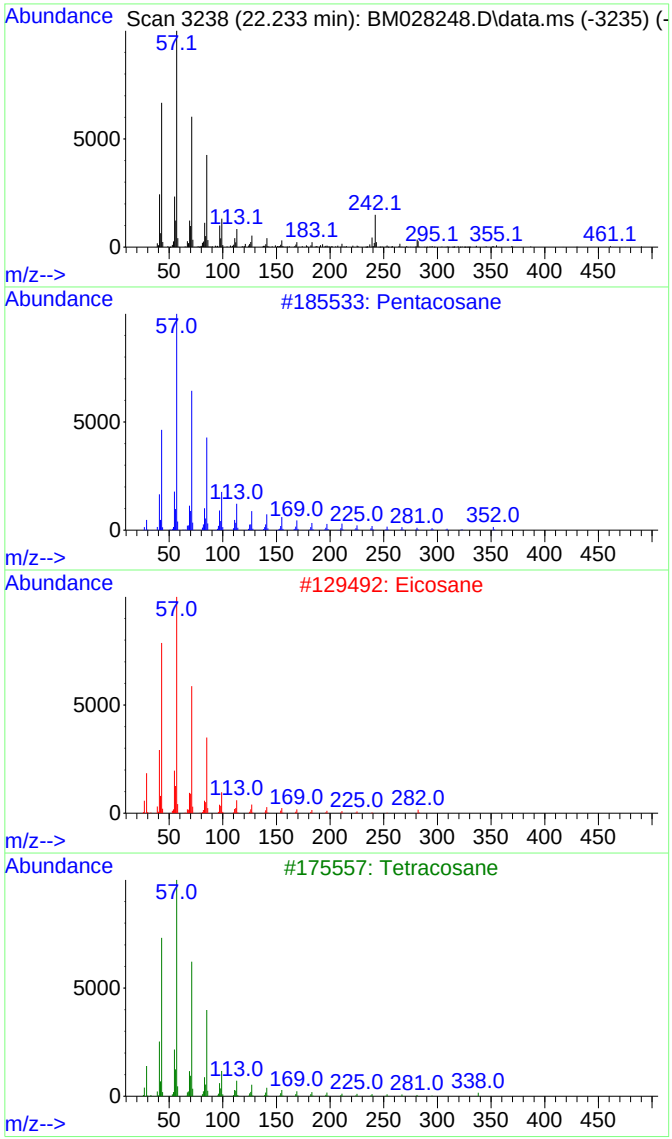
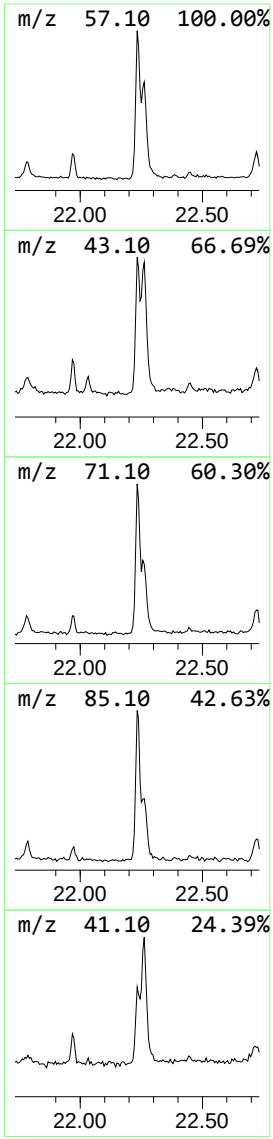
Peak Number 6 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.233	2.84 ng	300939	Chrysene-d12	21.656

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	96
2	Eicosane	282	C20H42	000112-95-8	93
3	Tetracosane	338	C24H50	000646-31-1	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptacosane	380	C27H56	000593-49-7	87





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Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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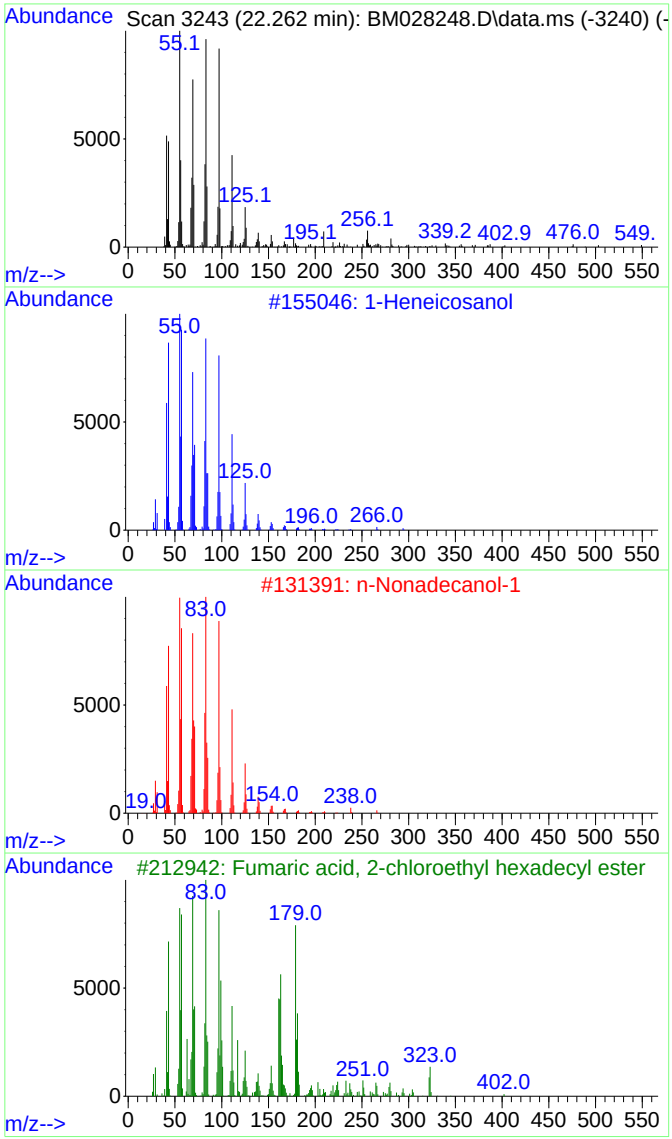
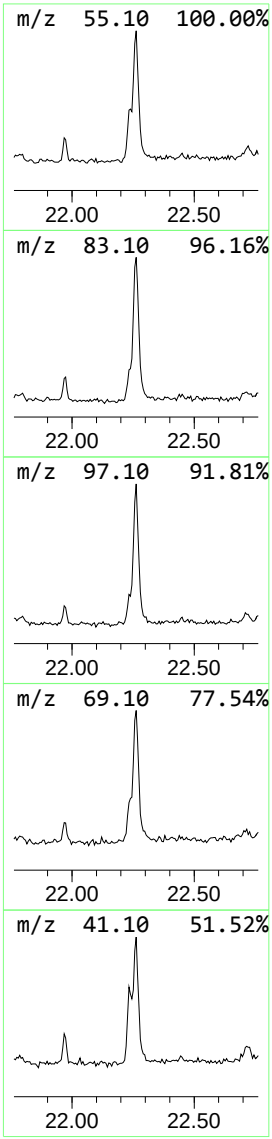
Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.262	5.67 ng	600871	Chrysene-d12	21.656

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	86
3	Fumaric acid, 2-chloroethyl hexa...	402	C22H39ClO4	1000330-62-2	80
4	4,4-Dimethylpent-2-enal	112	C7H12O	1000195-01-6	53
5	Cyclopentadecane	210	C15H30	000295-48-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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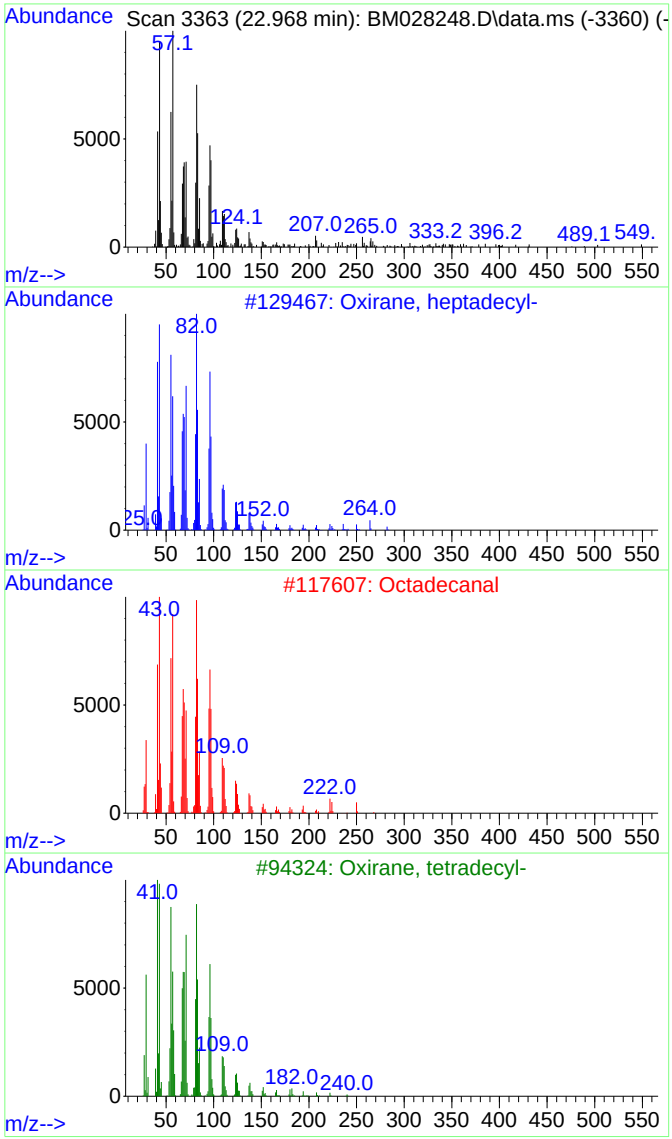
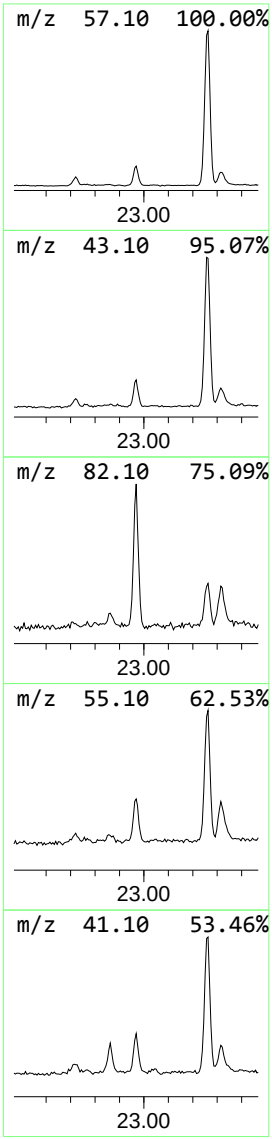
Peak Number 8 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.968	4.52 ng	277132	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	83
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
5	Tetradecanal	212	C14H28O	000124-25-4	74





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Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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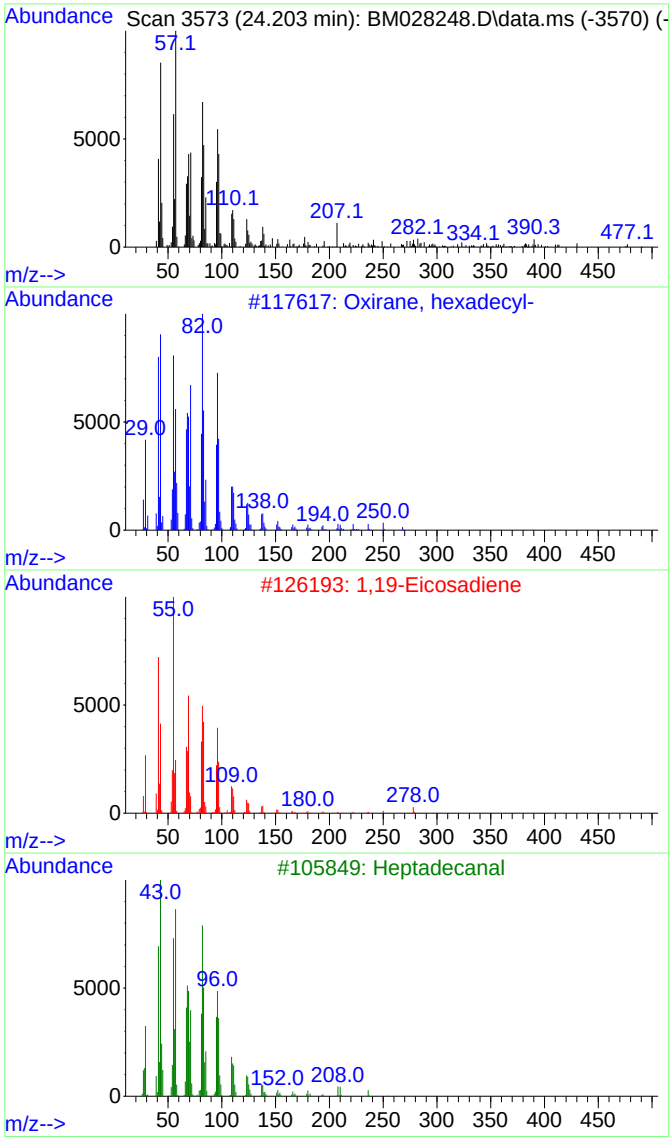
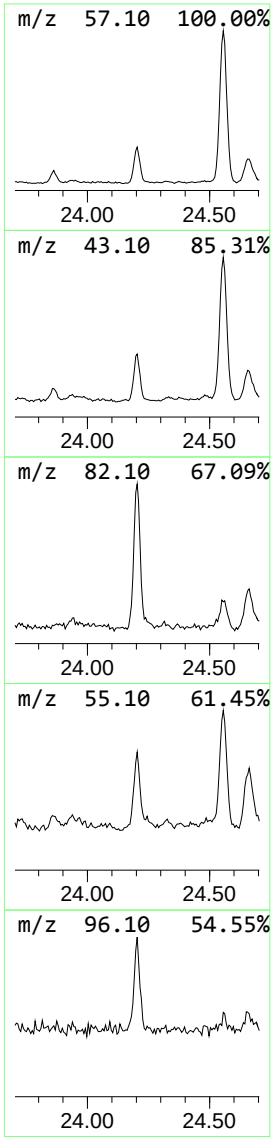
Peak Number 9 Oxirane, hexadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.203	4.91 ng	301548	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2	1,19-Eicosadiene	278	C20H38	014811-95-1	92
3	Heptadecanal	254	C17H34O	1000376-70-0	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
5	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	83





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Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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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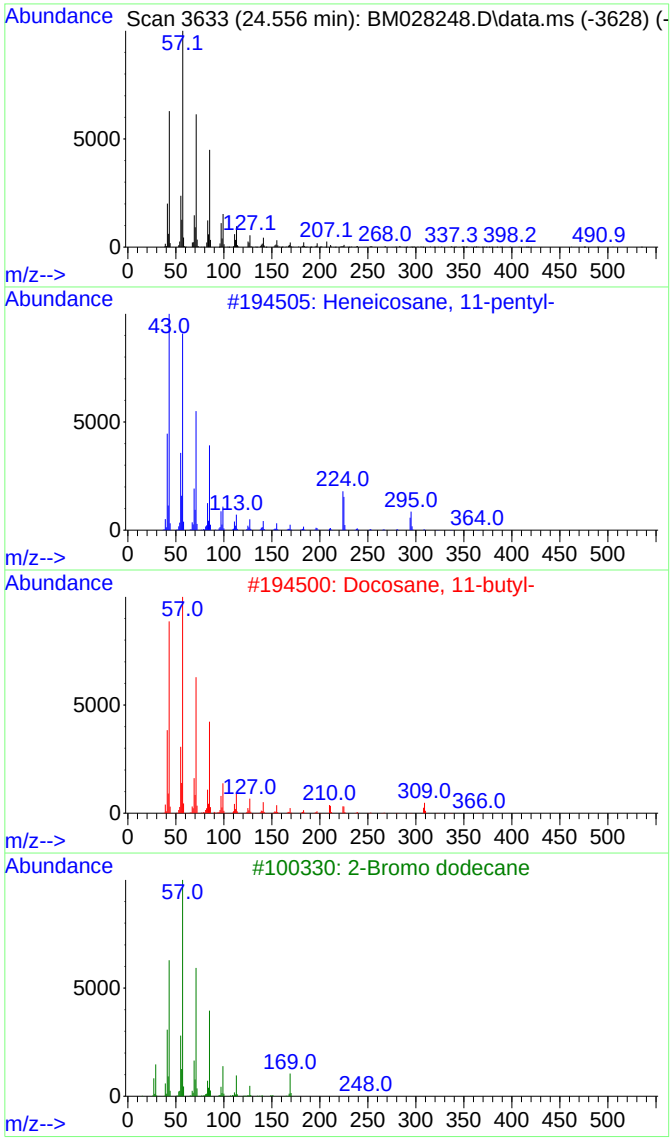
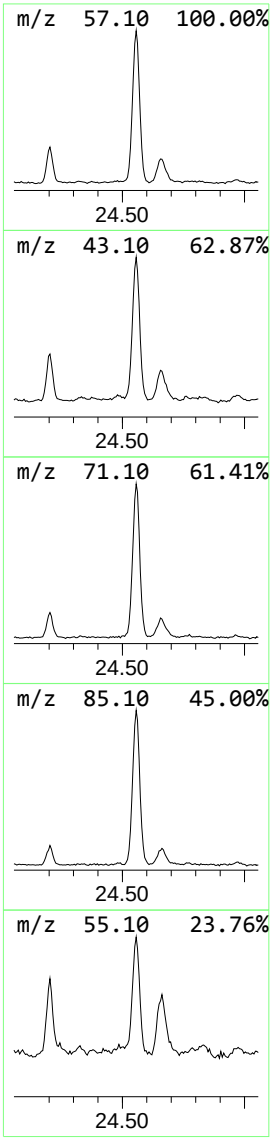
Peak Number 10 Heneicosane, 11-pentyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.556	16.41 ng	1006800	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122320\
Data File : BM028248.D
Acq On : 23 Dec 2020 12:59
Operator : JU/CG
Sample : L5176-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CHRT-27339

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.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
Ethanol, 2-(2-e...	7.775	3.8	ng	148924	1	8.193	794742	20.0
2,4,7,9-Tetrame...	13.704	17.2	ng	1038600	3	14.822	1210160	20.0
unknown15.91	15.910	3.7	ng	221256	3	14.822	1210160	20.0
n-Hexadecanoic ...	18.398	4.7	ng	314341	4	17.545	1332120	20.0
3-Eicosene, (E)-	21.345	5.4	ng	568802	5	21.656	2118560	20.0
Pentacosane	22.233	2.8	ng	300939	5	21.656	2118560	20.0
1-Heneicosanol	22.262	5.7	ng	600871	5	21.656	2118560	20.0
Oxirane, heptad...	22.968	4.5	ng	277132	6	24.027	1227140	20.0
Oxirane, hexade...	24.203	4.9	ng	301548	6	24.027	1227140	20.0
Heneicosane, 11...	24.556	16.4	ng	1006800	6	24.027	1227140	20.0