LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047243.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	62	65	74	rBV	141875	188088	3.04%	0.289%
2	4.581	281	288	297	rVB	155868	226402	3.65%	0.348%
3	5.022	357	363	373	rBV	2264639	3280490	52.96%	5.036%
4	6.581	622	628	643	rBV	2106168	3383155	54.62%	5.194%
5	7.004	696	700	709	rBV	43569	92833	1.50%	0.143%
6	7.369	755	762	771	rBV	1137245	1728575	27.90%	2.654%
7	8.516	949	957	969	rBV	1442112	2311421	37.31%	3.549%
8	9.092	1051	1055	1067	rBV4	31896	70438	1.14%	0.108%
9	10.128	1221	1231	1237	rBV	1353416	2270330	36.65%	3.486%
10	10.886	1354	1360	1370	rBV	162534	323237	5.22%	0.496%
11	11.839	1517	1522	1533	rBV	109138	222837	3.60%	0.342%
12	12.633	1650	1657	1666	rBV	3501235	5195348	83.87%	7.976%
13	13.745	1843	1846	1851	rVB	68523	103325	1.67%	0.159%
14	14.027	1888	1894	1900	rVV	1988929	2949481	47.61%	4.528%
15	14.092	1900	1905	1914	rVB2	100186	206240	3.33%	0.317%
16	14.263	1928	1934	1935	rBV3	65806	91854	1.48%	0.141%
17	14.286	1935	1938	1944	rVB4	82087	146788	2.37%	0.225%
18	14.368	1947	1952	1956	rBV2	58295	100281	1.62%	0.154%
19	14.580	1984	1988	1995	rVB6	41750	70589	1.14%	0.108%
20	14.921	2042	2046	2050	rBV2	126249	157979	2.55%	0.243%
21	15.092	2070	2075	2079	rBV	90051	132552	2.14%	0.203%
22	15.421	2128	2131	2137	rVB4	97142	143017	2.31%	0.220%
23	15.539	2145	2151	2160	rBV	2868551	4003436	64.63%	6.146%
24	15.792	2190	2194	2202	rVB2	238835	480260	7.75%	0.737%
25	16.339	2283	2287	2290	rBV	126884	172075	2.78%	0.264%
26	16.586	2325	2329	2332	rBV	214922	274167	4.43%	0.421%
27	16.639	2335	2338	2343	rVB	115946	169734	2.74%	0.261%
28	16.792	2359	2364	2368	rBV	2348466	3329481	53.75%	5.112%
29	16.833	2368	2371	2376	rVB	943536	1233384	19.91%	1.894%
30	16.927	2382	2387	2391	rVB	297286	421178	6.80%	0.647%
31	17.327	2451	2455	2459	rBV2	235889	276777	4.47%	0.425%
32	17.374	2460	2463	2467	rVV2	68387	92827	1.50%	0.143%
33	17.504	2480	2485	2493	rVB	899837	1146461	18.51%	1.760%
34	17.674	2510	2514	2518	rBV	181962	253021	4.08%	0.388%
35	17.727	2518	2523	2532	rBV2	1072168	1598985	25.81%	2.455%
36	17.862	2542	2546	2550	rBV2	313271	431397	6.96%	0.662%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.021	2570	2573	2577	rBV	216786	240783	3.89%	0.370%
38	18.186	2597	2601	2604	rBV	118397	187174	3.02%	0.287%
39	18.656	2676	2681	2684	rBV	3230269	4043927	65.28%	6.208%
40	18.692	2684	2687	2691	rVB2	2256564	2668807	43.08%	4.097%
41	18.827	2707	2710	2713	rBV	609036	666726	10.76%	1.024%
42	18.868	2713	2717	2722	rBV	1938444	2561773	41.36%	3.933%
43	19.027	2741	2744	2751	rBV3	349125	523366	8.45%	0.803%
44	19.233	2772	2779	2790	rBV	1648969	3034231	48.98%	4.658%
45	19.462	2813	2818	2822	rVB	5149497	6194552	100.00%	9.510%
46	21.033	3079	3085	3089	rBV2	2432843	4087732	65.99%	6.276%
47	23.744	3542	3546	3563	rVB	1525603	3648820	58.90%	5.602%

Sum of corrected areas: 65136334

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Instrument :
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ClientSampleId :
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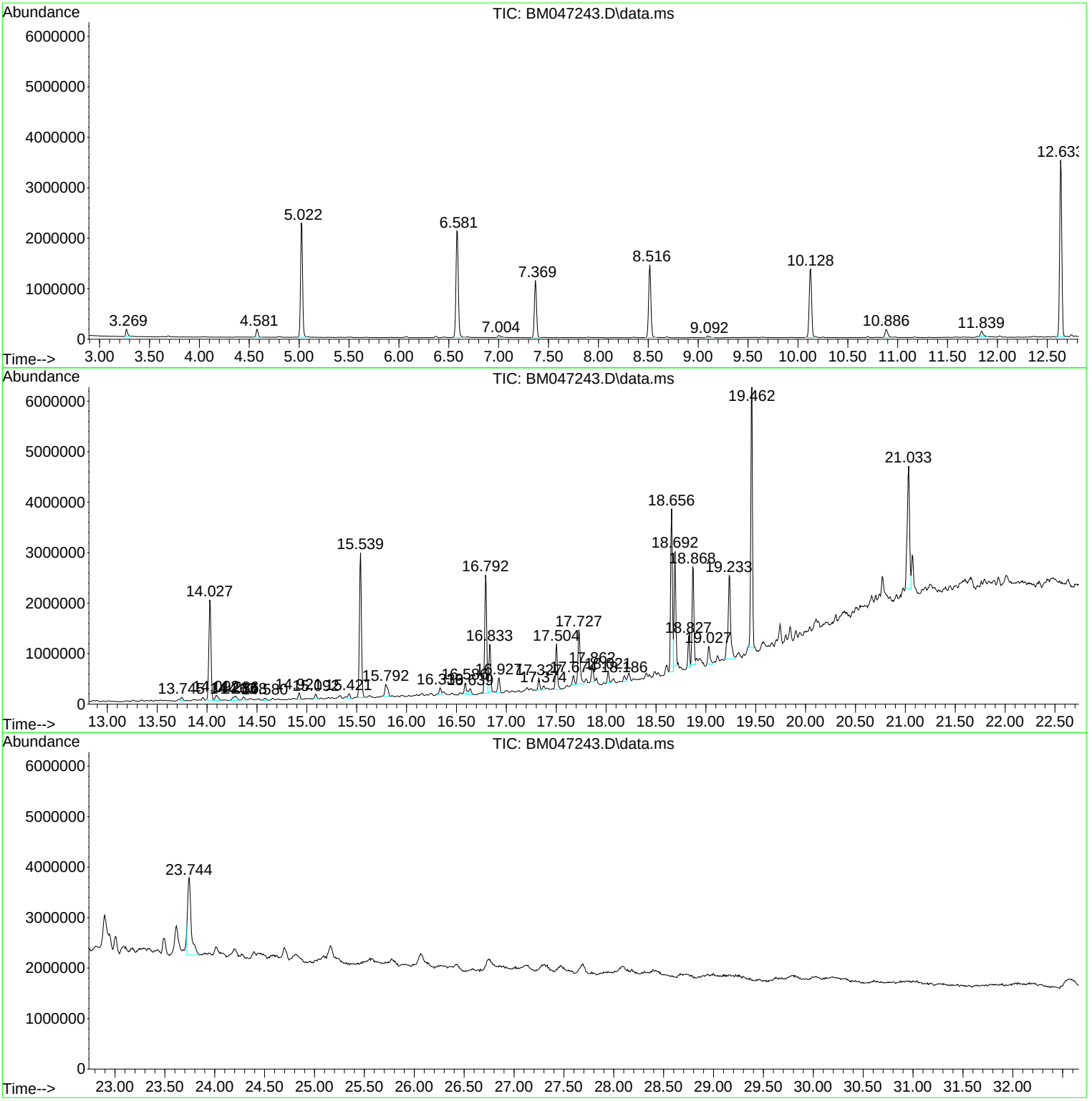
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

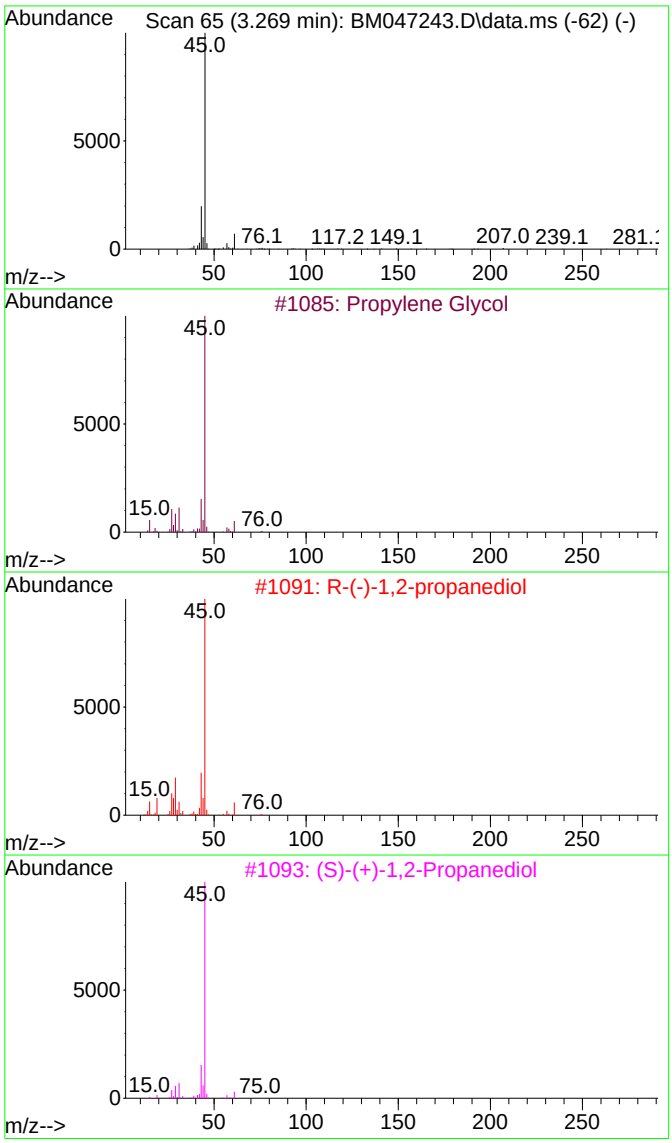
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

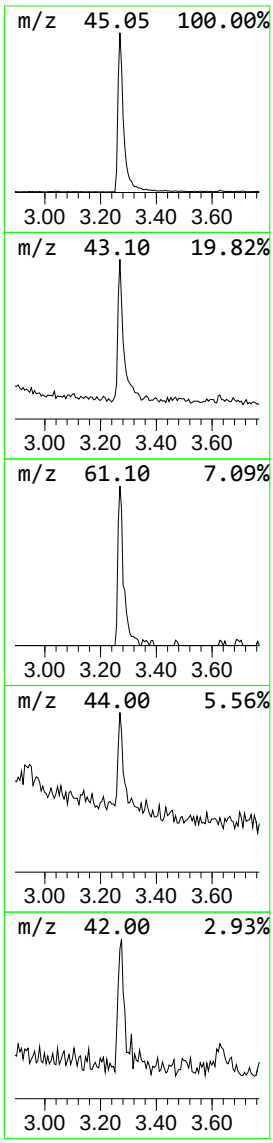
****

Peak Number 1 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.269	2.18 ng	188088	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	72
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





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Data File : BM047243.D
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Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

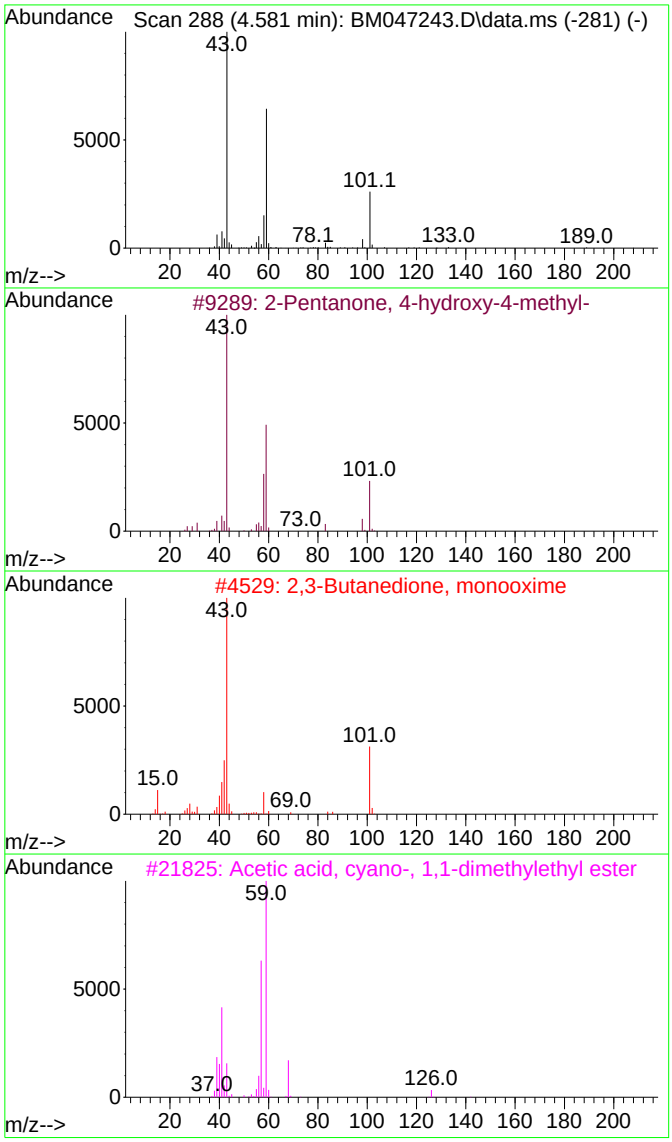
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

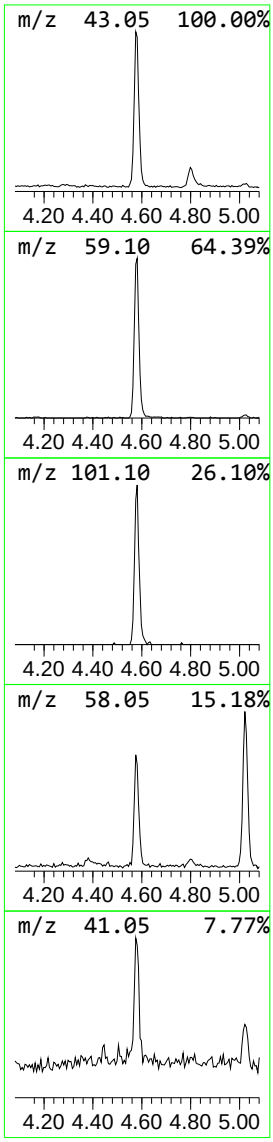
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.581	2.62 ng	226402	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
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Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

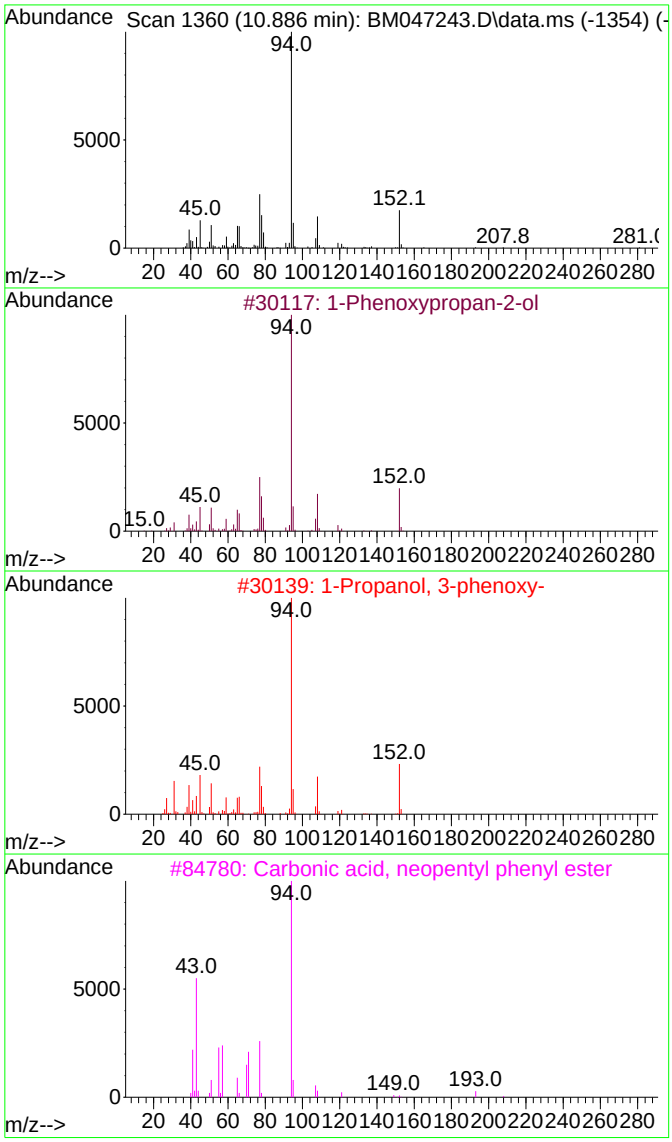
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

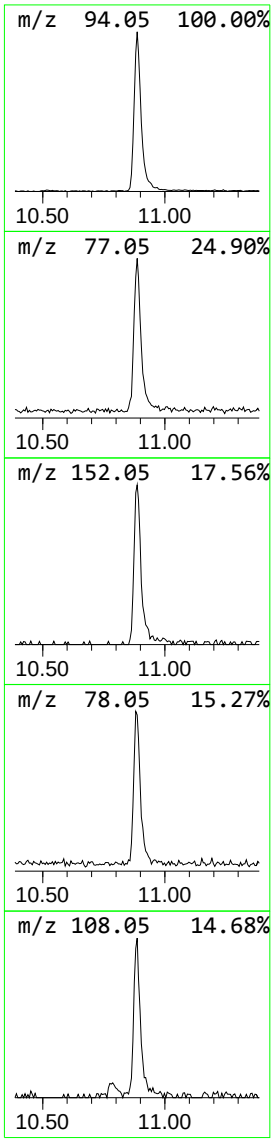
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.886	2.85 ng	323237	Naphthalene-d8	10.128

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	93
3	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

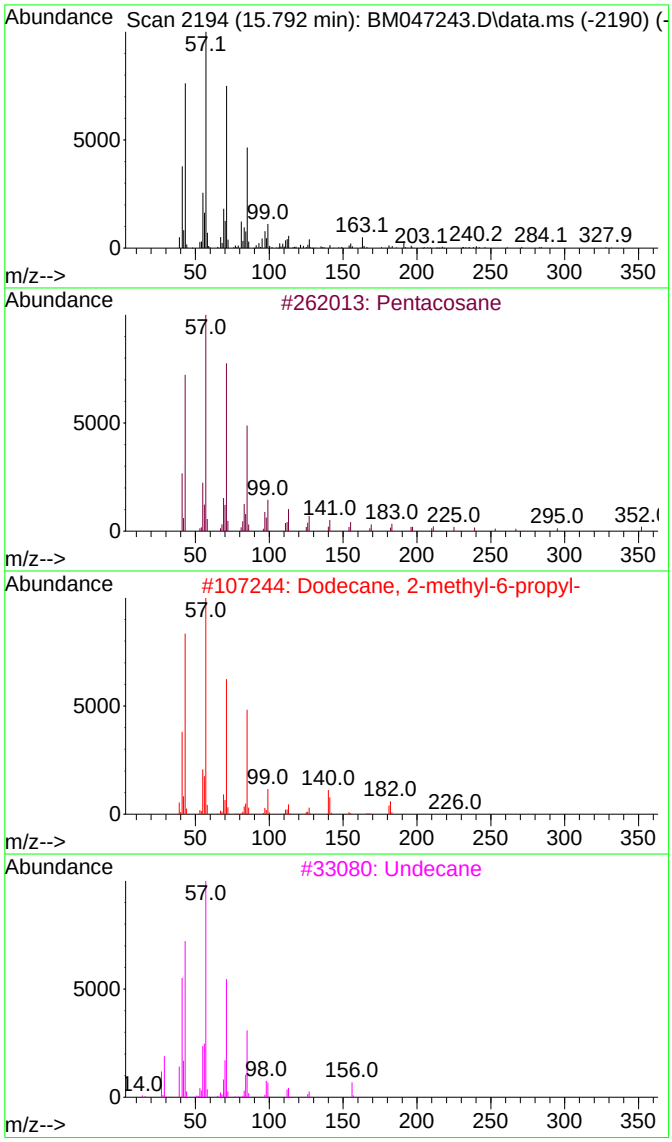
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

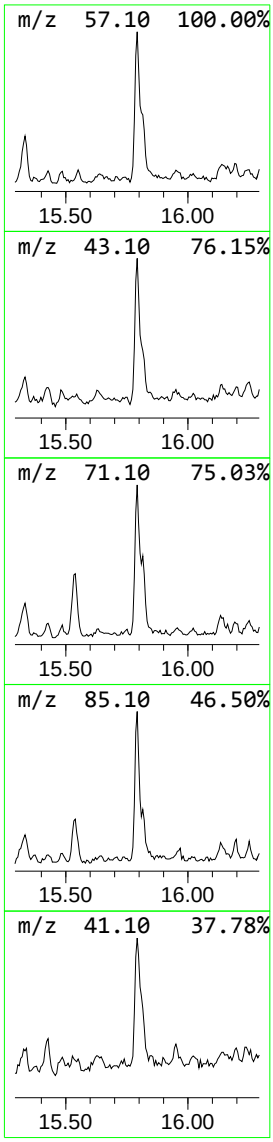
****

Peak Number 4 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	2.88 ng	480260	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
3	Undecane	156	C11H24	001120-21-4	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

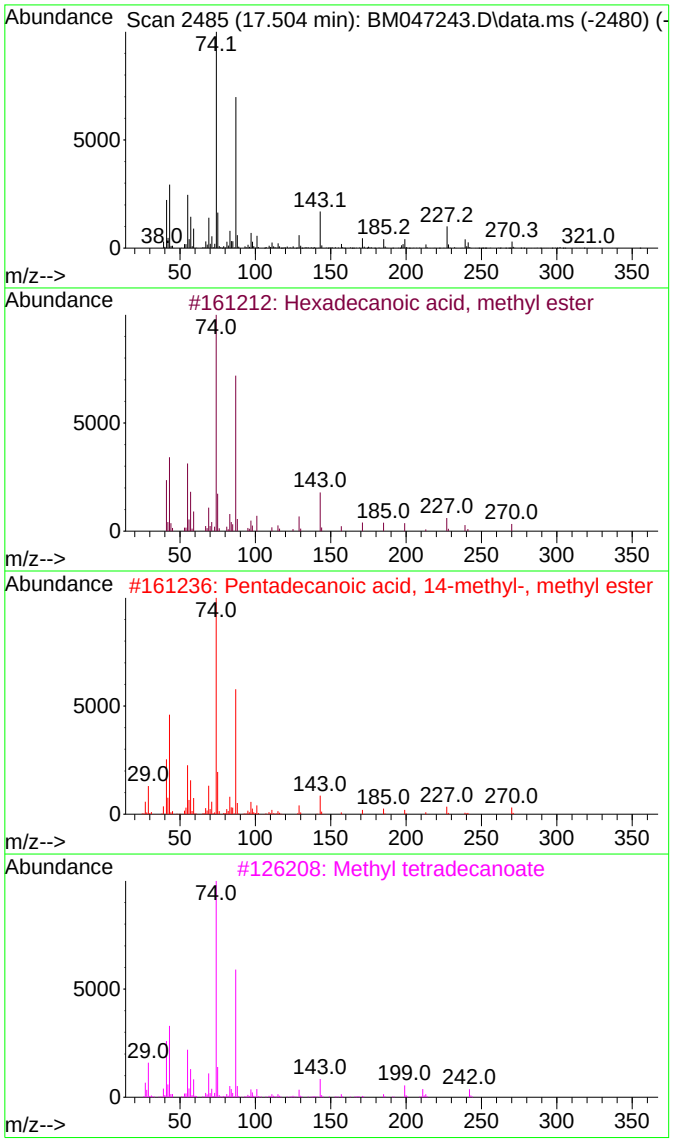
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

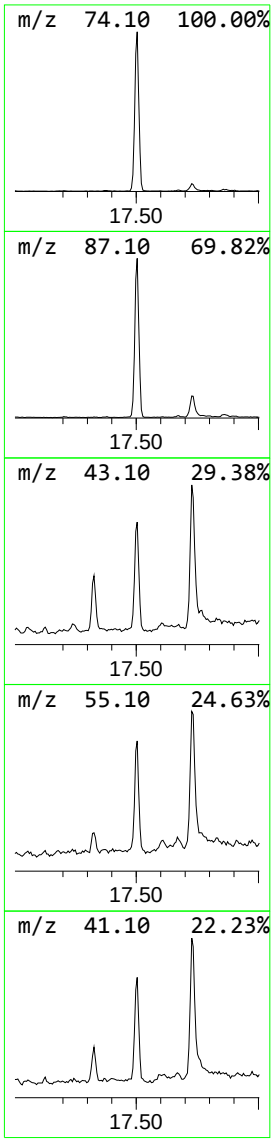
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.504	6.89 ng	1146460	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87





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Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

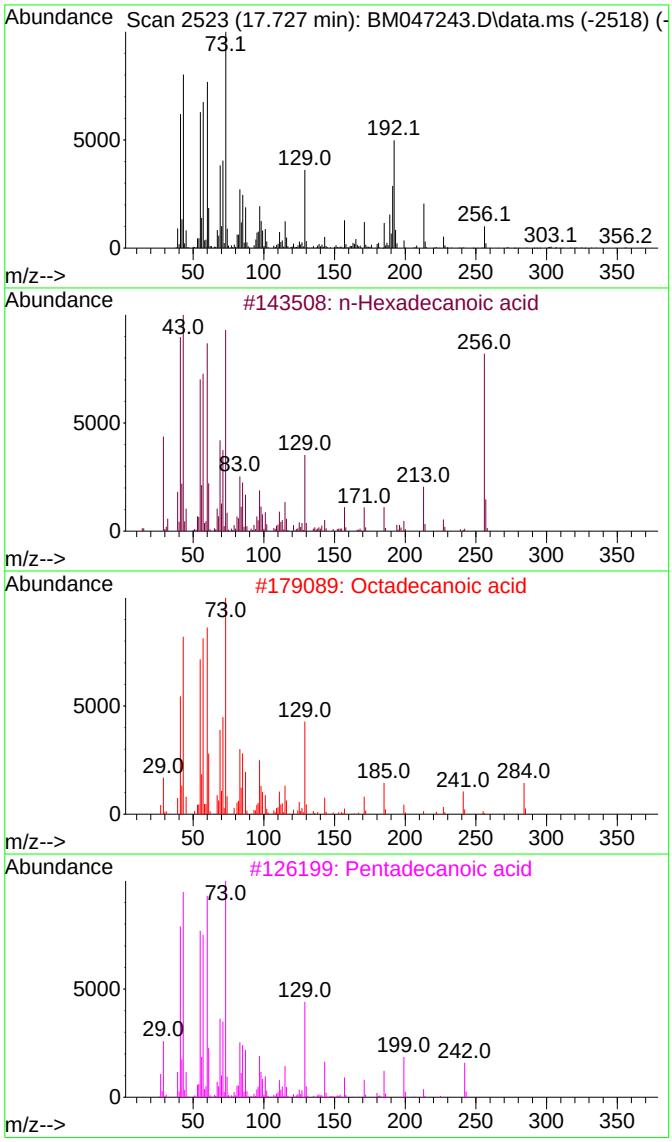
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

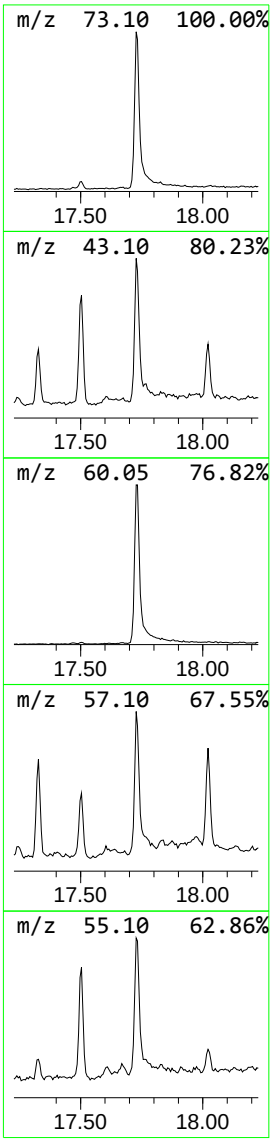
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	9.61 ng	1598990	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38





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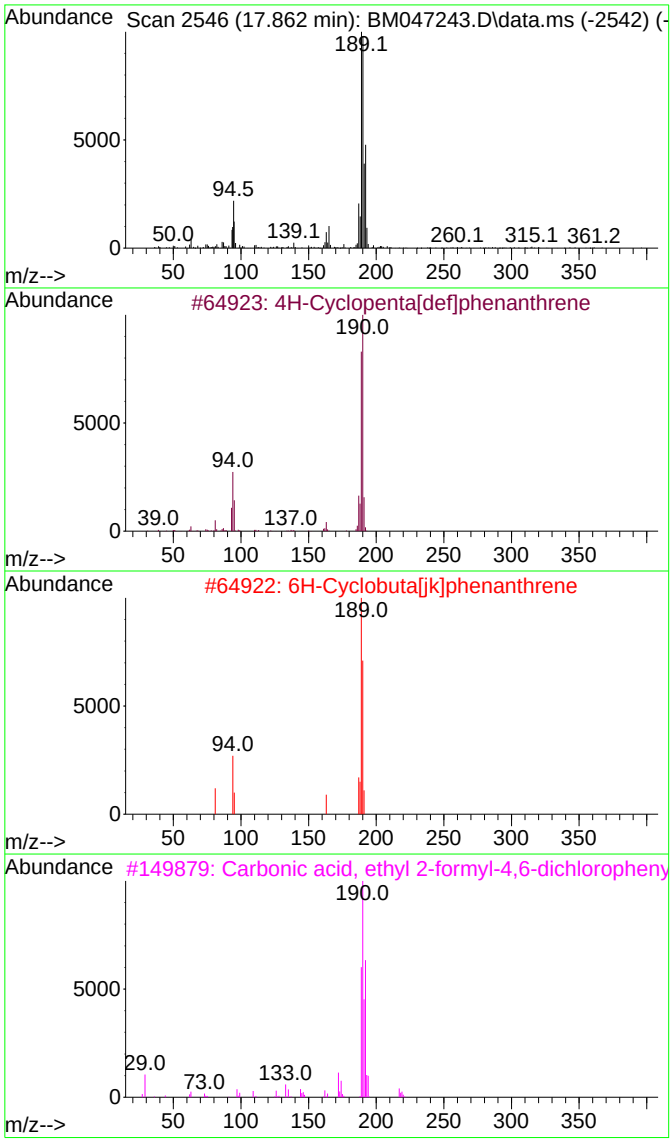
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

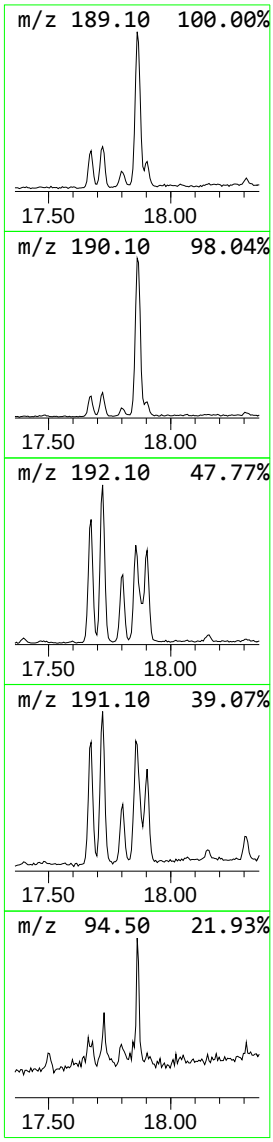
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.862	2.59 ng	431397	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	32





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Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

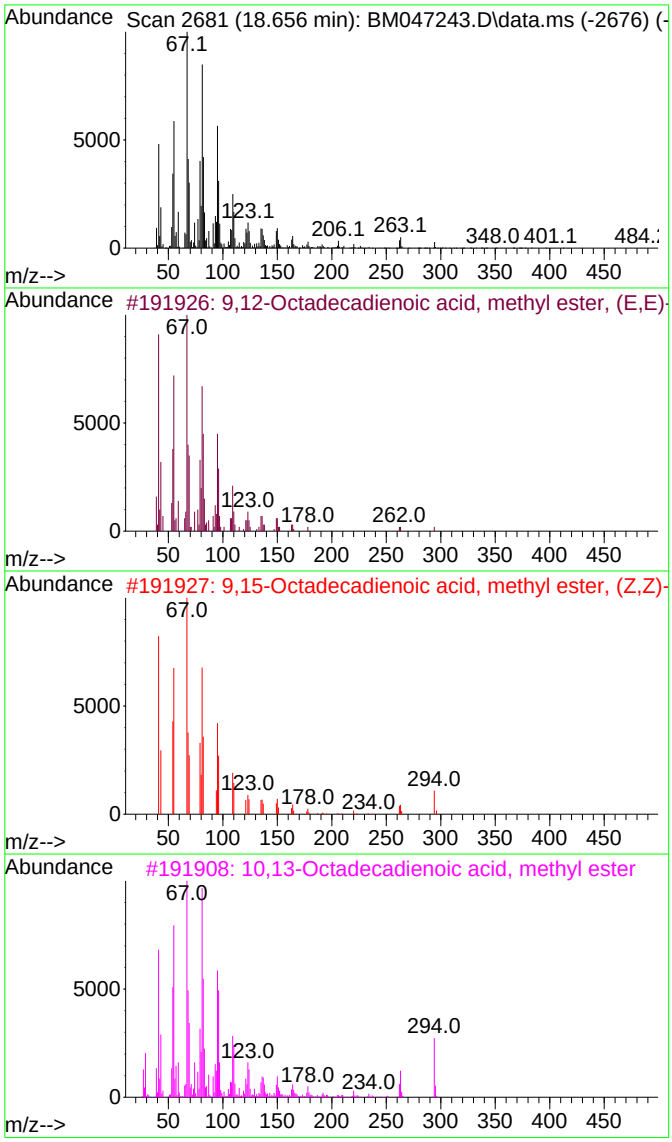
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

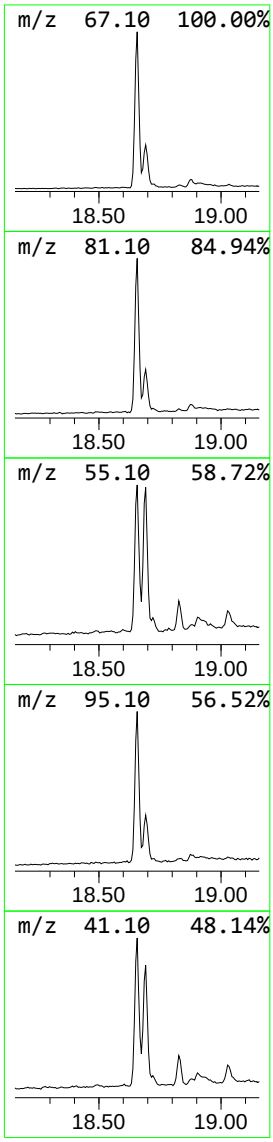
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.656	24.29 ng	4043930	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

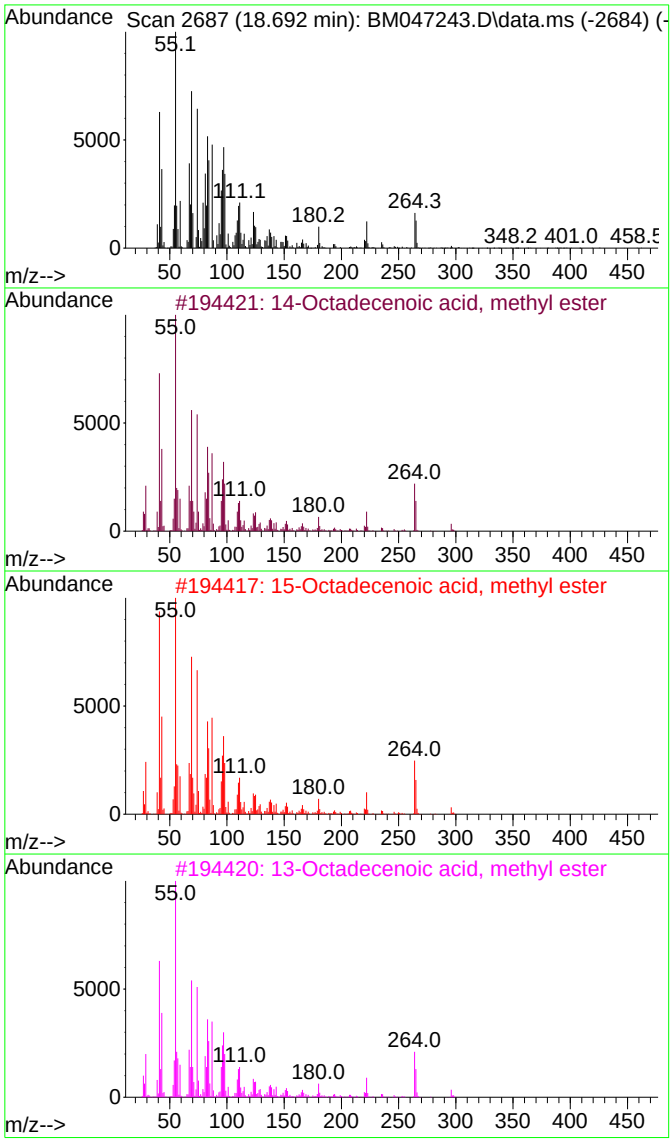
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

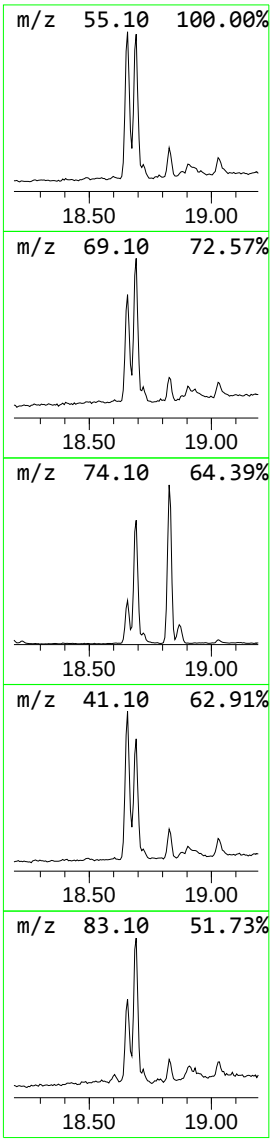
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 14-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.692	16.03 ng	2668810	Phenanthrene-d10	16.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

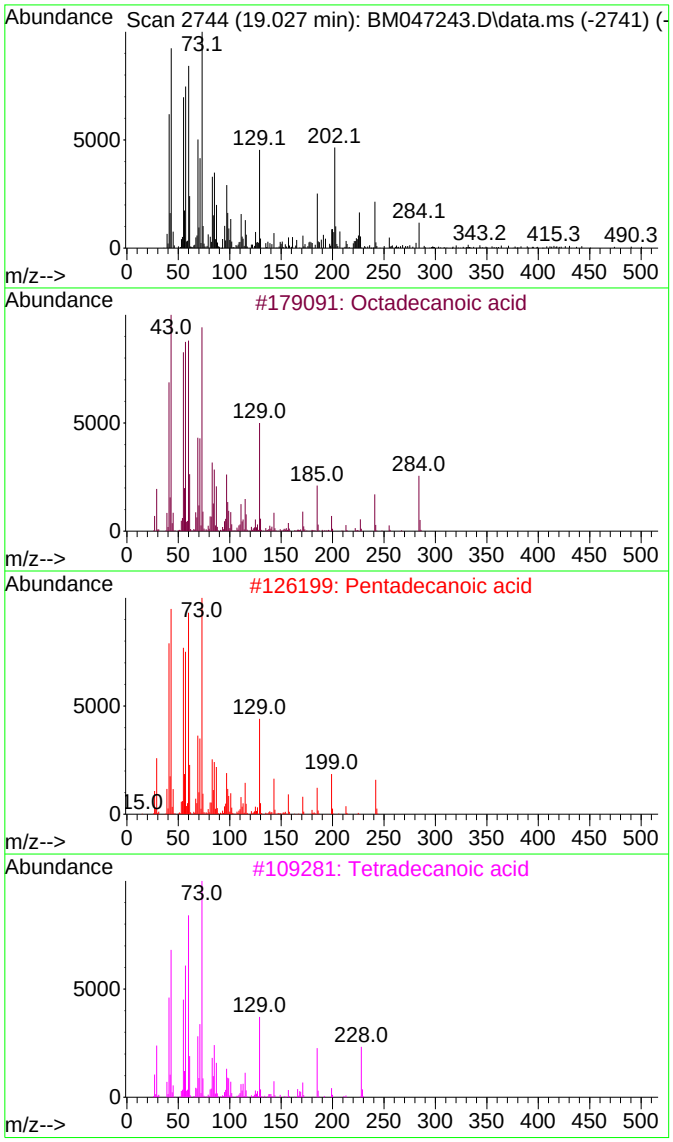
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

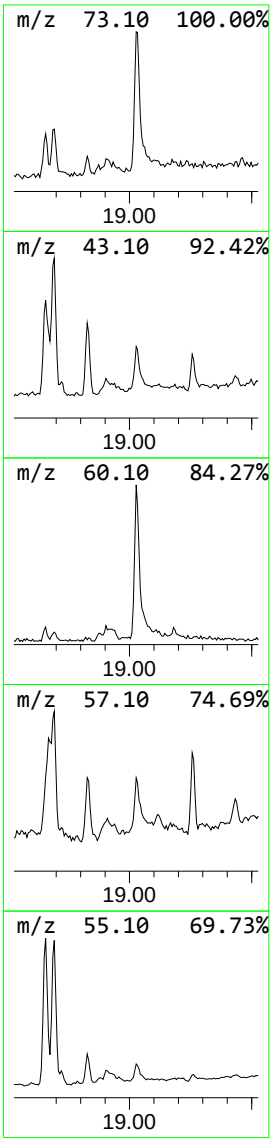
****

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	2.56 ng	523366	Chrysene-d12	21.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047243.D
Acq On : 16 Aug 2024 20:32
Operator : RC/JU
Sample : P3634-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-06-08152024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
Propylene Glycol	3.269	2.2	ng	188088	1	7.369	1728580	20.0
2-Pentanone, 4-...	4.581	2.6	ng	226402	1	7.369	1728580	20.0
1-Phenoxypropan...	10.886	2.9	ng	323237	2	10.128	2270330	20.0
Pentacosane	15.792	2.9	ng	480260	4	16.792	3329480	20.0
Hexadecanoic ac...	17.504	6.9	ng	1146460	4	16.792	3329480	20.0
n-Hexadecanoic ...	17.727	9.6	ng	1598990	4	16.792	3329480	20.0
4H-Cyclopenta[d...	17.862	2.6	ng	431397	4	16.792	3329480	20.0
9,12-Octadecadi...	18.656	24.3	ng	4043930	4	16.792	3329480	20.0
14-Octadecenoic...	18.692	16.0	ng	2668810	4	16.792	3329480	20.0
Octadecanoic acid	19.027	2.6	ng	523366	5	21.033	4087730	20.0