LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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: BM047317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	59	63	74	rBV	227983	325526	4.08%	0.578%
2	4.563	279	285	294	rBV	199708	286553	3.59%	0.509%
3	5.010	355	361	376	rBV	2992178	4289971	53.71%	7.623%
4	6.569	619	626	638	rBV	2873050	4568029	57.19%	8.117%
5	6.987	693	697	710	rBV	62883	124010	1.55%	0.220%
6	7.351	751	759	770	rBV	941877	1432646	17.94%	2.546%
7	7.651	803	810	817	rBV	308615	460135	5.76%	0.818%
8	8.498	941	954	967	rBV	1863527	3077253	38.52%	5.468%
9	9.086	1049	1054	1064	rBV2	47138	88967	1.11%	0.158%
10	10.104	1220	1227	1240	rBV	1187781	1945559	24.36%	3.457%
11	10.875	1350	1358	1372	rBV	132774	337333	4.22%	0.599%
12	12.616	1647	1654	1673	rBV	3809687	5866616	73.44%	10.424%
13	14.010	1884	1891	1902	rBV	1722315	2688730	33.66%	4.778%
14	14.268	1926	1935	1941	rBV4	175972	366517	4.59%	0.651%
15	15.521	2142	2148	2160	rBV	3593863	5269039	65.96%	9.362%
16	15.604	2160	2162	2175	rVB6	52077	106566	1.33%	0.189%
17	15.762	2184	2189	2194	rBV	67523	92295	1.16%	0.164%
18	16.345	2283	2288	2293	rBV4	47891	85922	1.08%	0.153%
19	16.774	2348	2361	2372	rBV	2266134	3471107	43.45%	6.168%
20	16.986	2391	2397	2405	rBV6	110378	265384	3.32%	0.472%
21	17.486	2478	2482	2485	rBV2	64959	88953	1.11%	0.158%
22	17.539	2486	2491	2509	rVB3	147987	418387	5.24%	0.743%
23	17.674	2509	2514	2517	rBV	397371	557574	6.98%	0.991%
24	17.709	2517	2520	2528	rVB	448334	607044	7.60%	1.079%
25	17.821	2535	2539	2548	rVB3	84402	139217	1.74%	0.247%
26	18.639	2674	2678	2683	rBV4	50485	91182	1.14%	0.162%
27	18.856	2711	2715	2719	rBV2	66038	103303	1.29%	0.184%
28	19.015	2737	2742	2753	rBV2	160552	284004	3.56%	0.505%
29	19.268	2781	2785	2798	rVB	272260	477858	5.98%	0.849%
30	19.374	2799	2803	2806	rBV2	53088	81225	1.02%	0.144%
31	19.445	2806	2815	2825	rVB	6426173	7987863	100.00%	14.193%
32	19.592	2836	2840	2846	rVB	110194	129497	1.62%	0.230%
33	19.892	2887	2891	2900	rVB5	60251	100666	1.26%	0.179%
34	20.750	3033	3037	3051	rBV	827411	1463013	18.32%	2.600%
35	21.015	3077	3082	3088	rBV	2696126	3487603	43.66%	6.197%
36	21.768	3205	3210	3221	rVB2	691921	1458429	18.26%	2.591%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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	22.974	3412	3415	3421	rVB	169005	262033	3.28%	0.466%
38	23.709	3532	3540	3555	rVB	1461477	3392457	42.47%	6.028%

Sum of corrected areas: 56278466

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
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Operator : RC/JU
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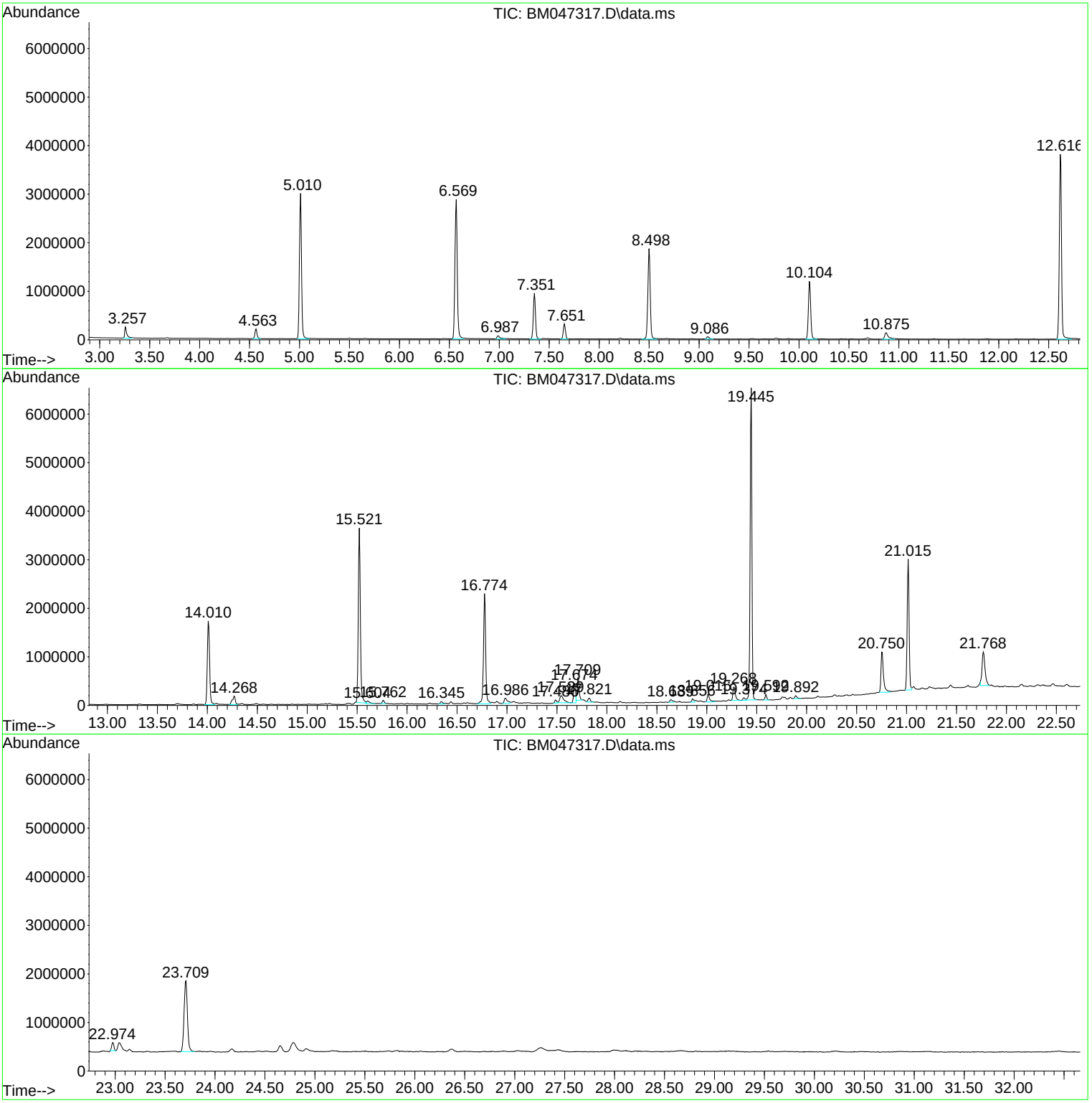
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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\BM082224\
Data File : BM047317.D
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Operator : RC/JU
Sample : P3671-10
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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

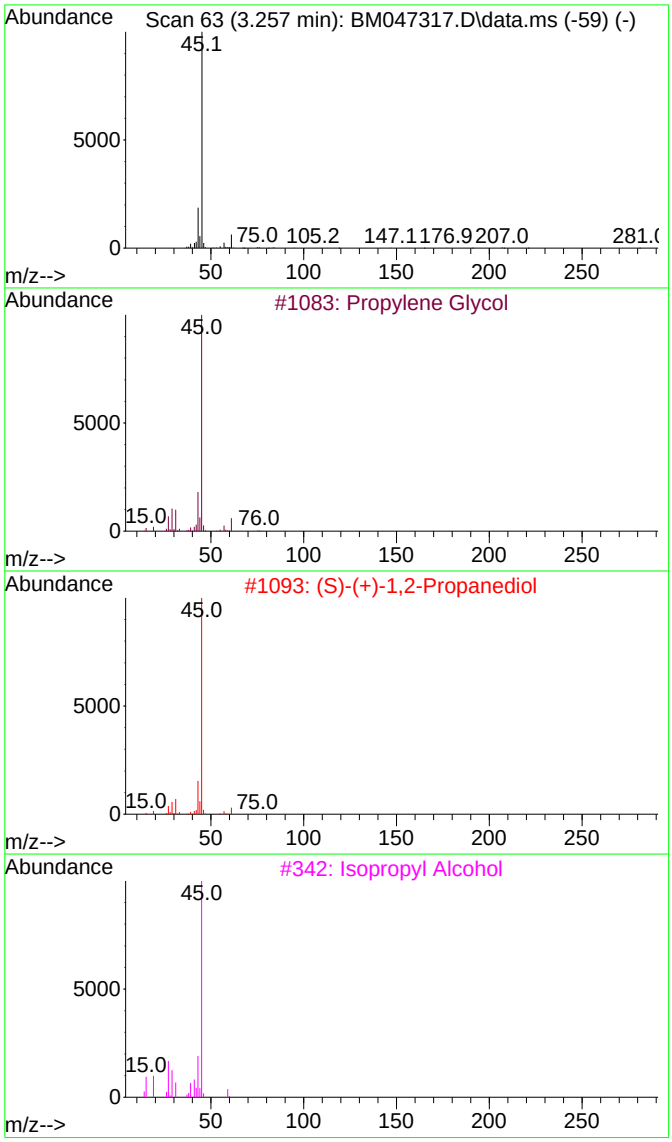
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

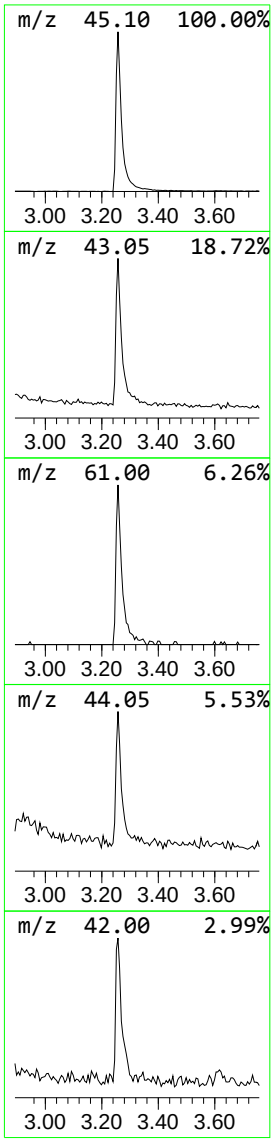
****

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	4.54 ng	325526	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

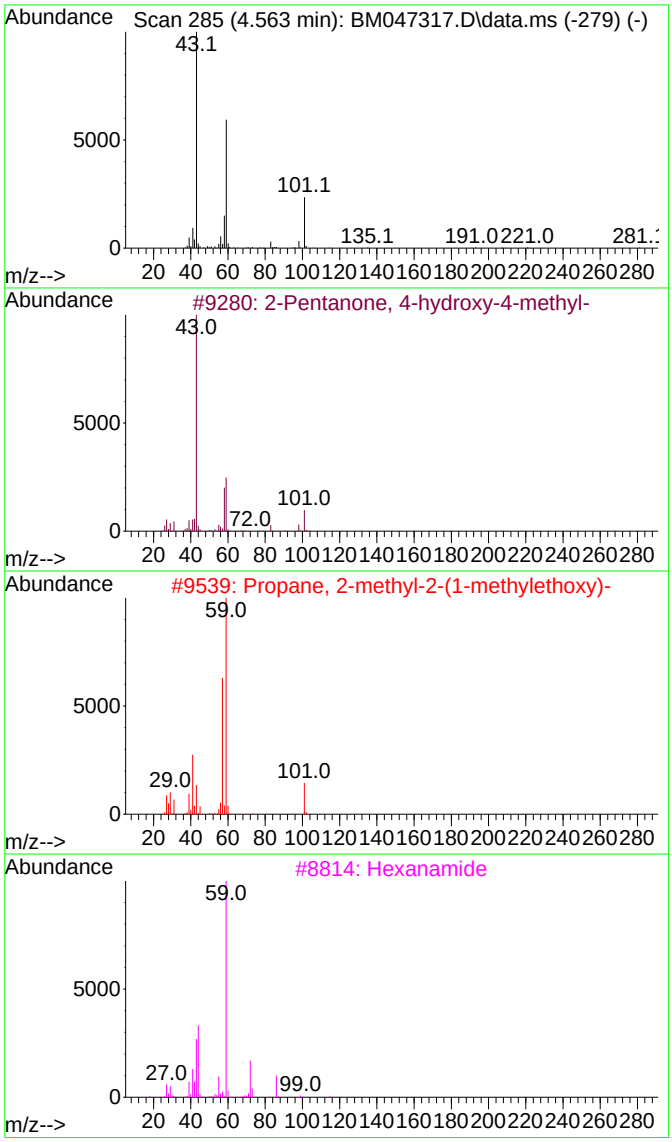
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

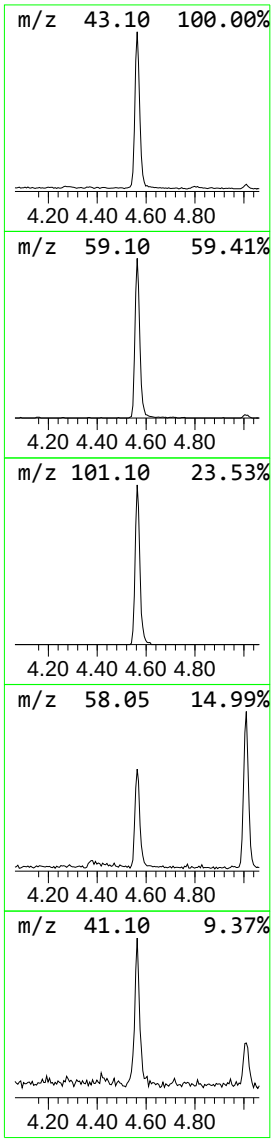
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	4.00 ng	286553	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	Hexanamide	115	C6H13NO	000628-02-4	16
4	Silane, dimethyl-	60	C2H8Si	001111-74-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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

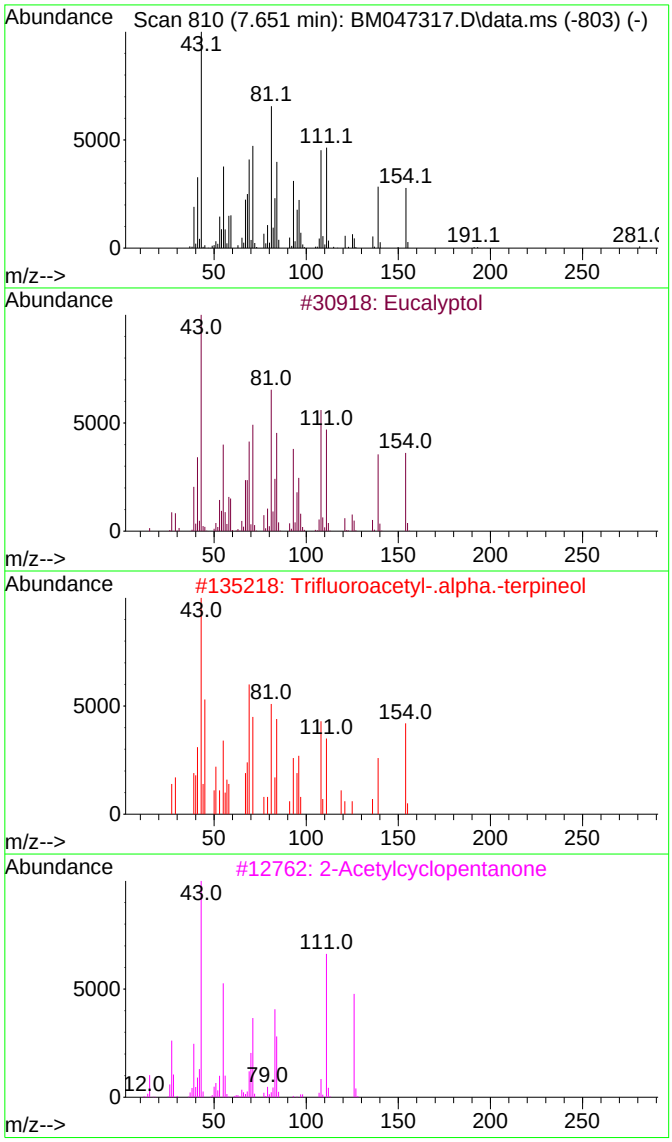
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

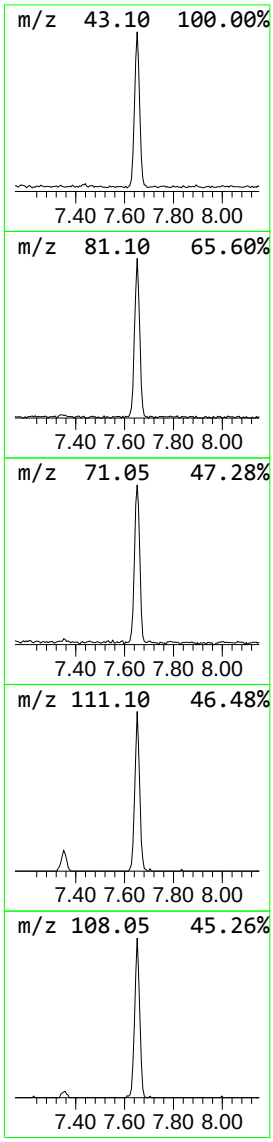
****

Peak Number 3 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	6.42 ng	460135	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4	1-Methylbicyclo[2.2.1]heptan-exo...	126	C8H14O	000766-25-6	25
5	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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

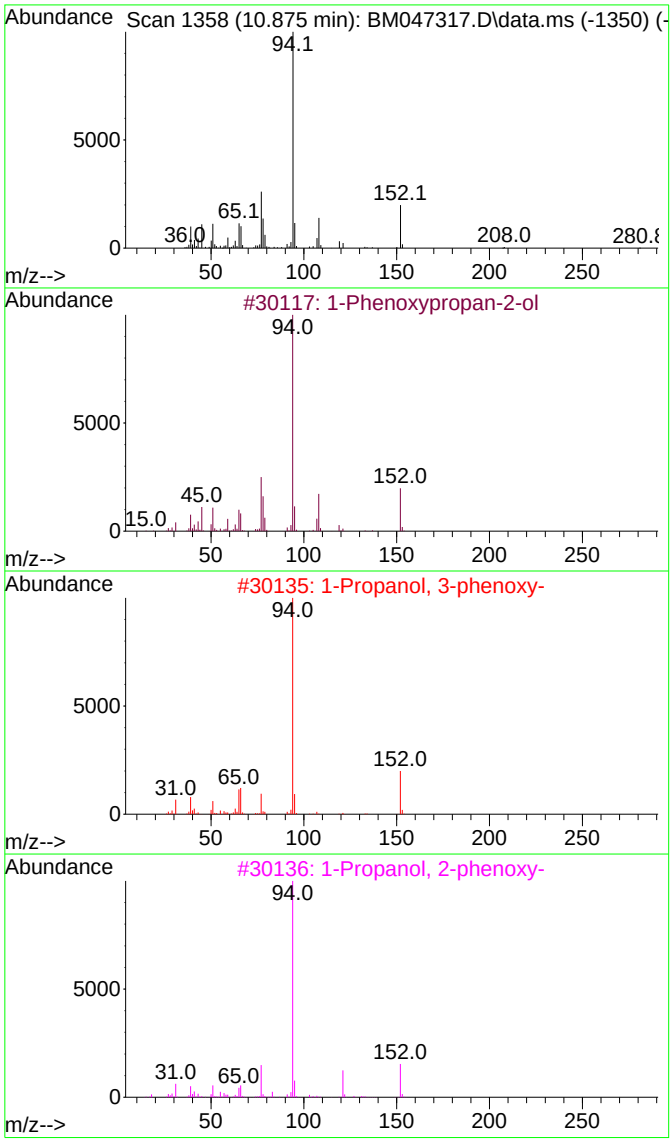
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

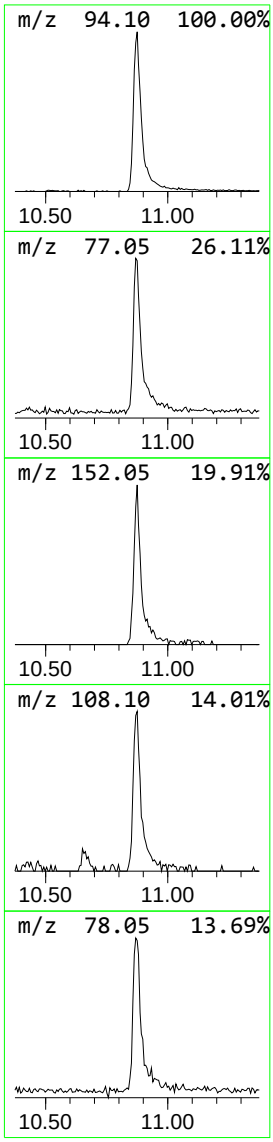
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.874	3.47 ng	337333	Naphthalene-d8	10.104

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	68
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

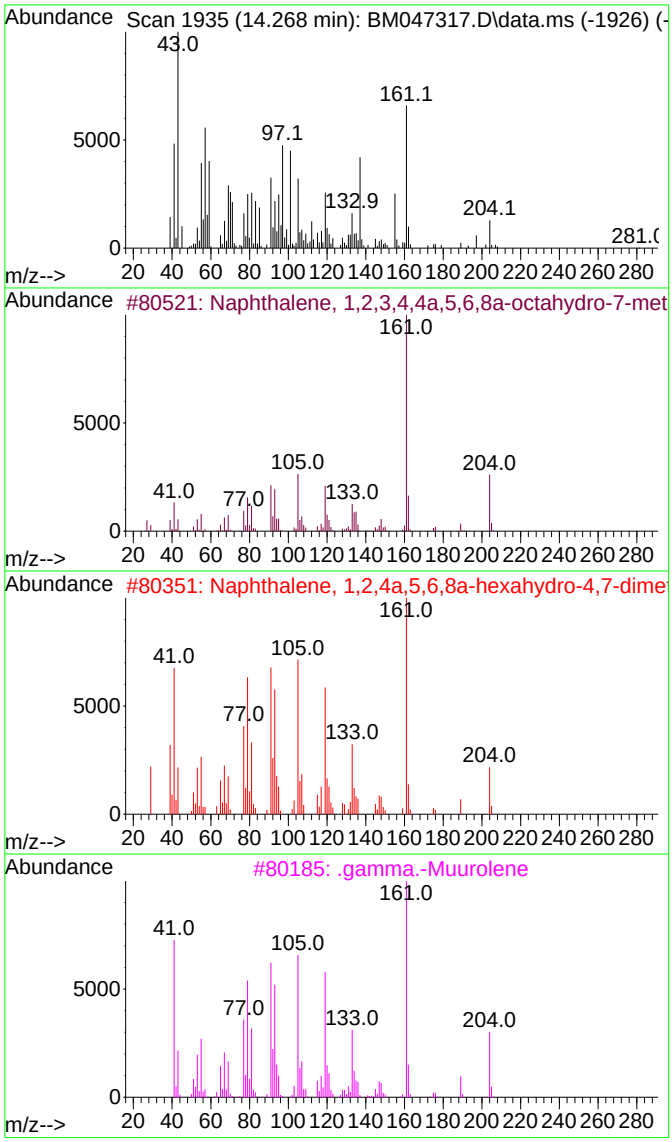
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

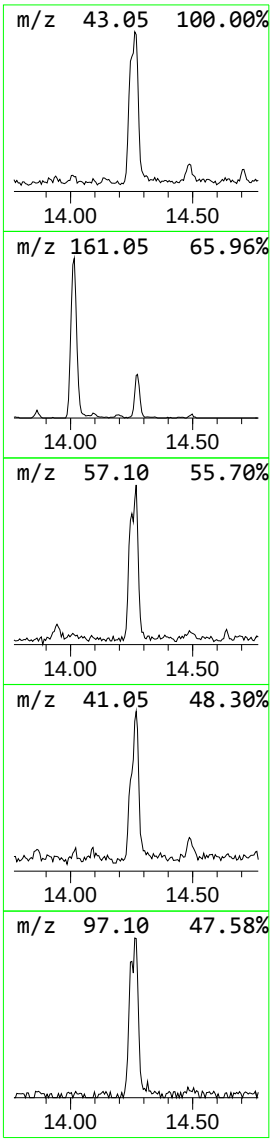
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	2.73 ng	366517	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	91
2	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	90
3	.gamma.-Muurolene	204	C15H24	030021-74-0	62
4	(S,1Z,6Z)-8-Isopropyl-1-methyl-5...	204	C15H24	317819-80-0	47
5	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	45





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Data File : BM047317.D
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Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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
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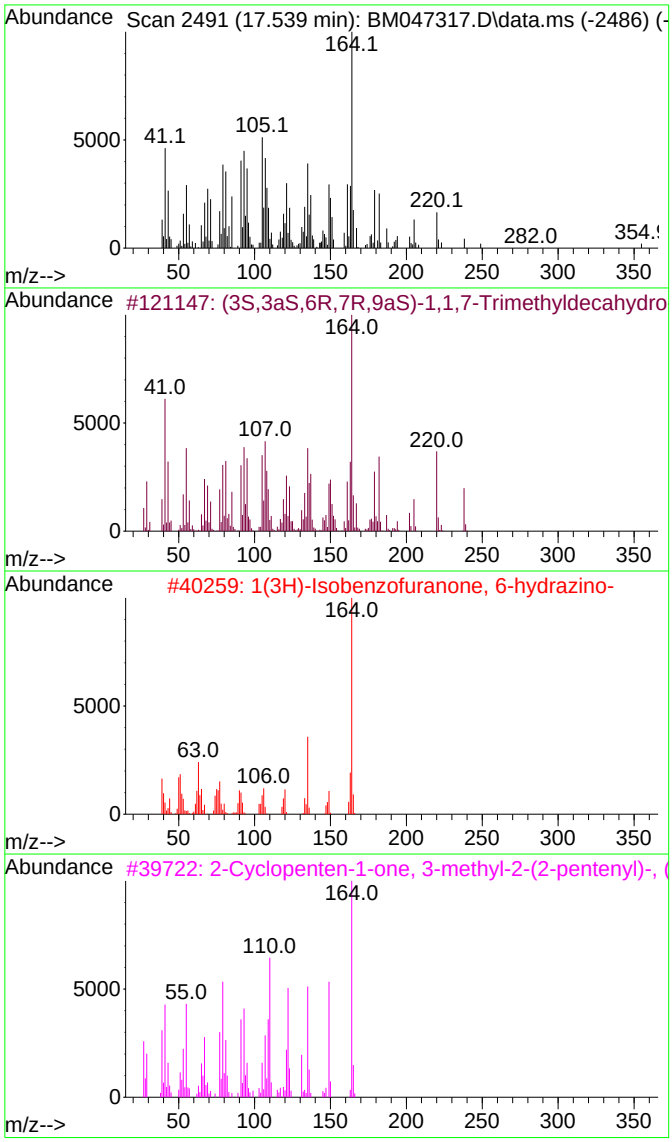
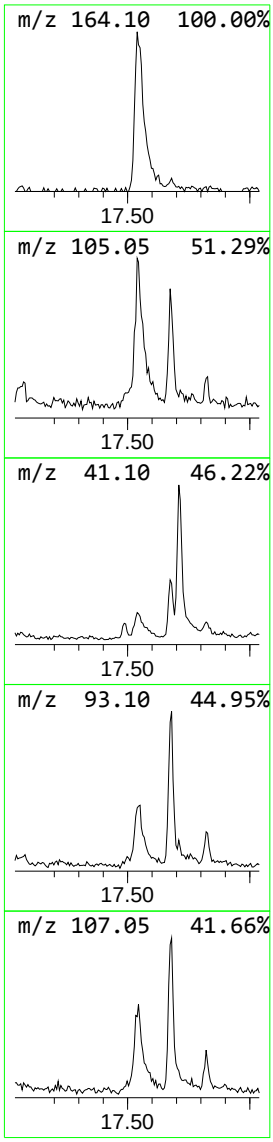
****
Peak Number 6 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.539	2.41 ng	418387	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	96
2	1(3H)-Isobenzofuranone, 6-hydraz...	164	C8H8N2O2	1000362-60-8	38
3	2-Cyclopenten-1-one, 3-methyl-2-...	164	C11H16O	000488-10-8	35
4	6-Methyl-7,8-dihydro-2(1H)-pteri...	164	C7H8N4O	089852-89-1	35
5	2,3,5,6-Tetramethyl-para-phenyle...	164	C10H16N2	003102-87-2	30





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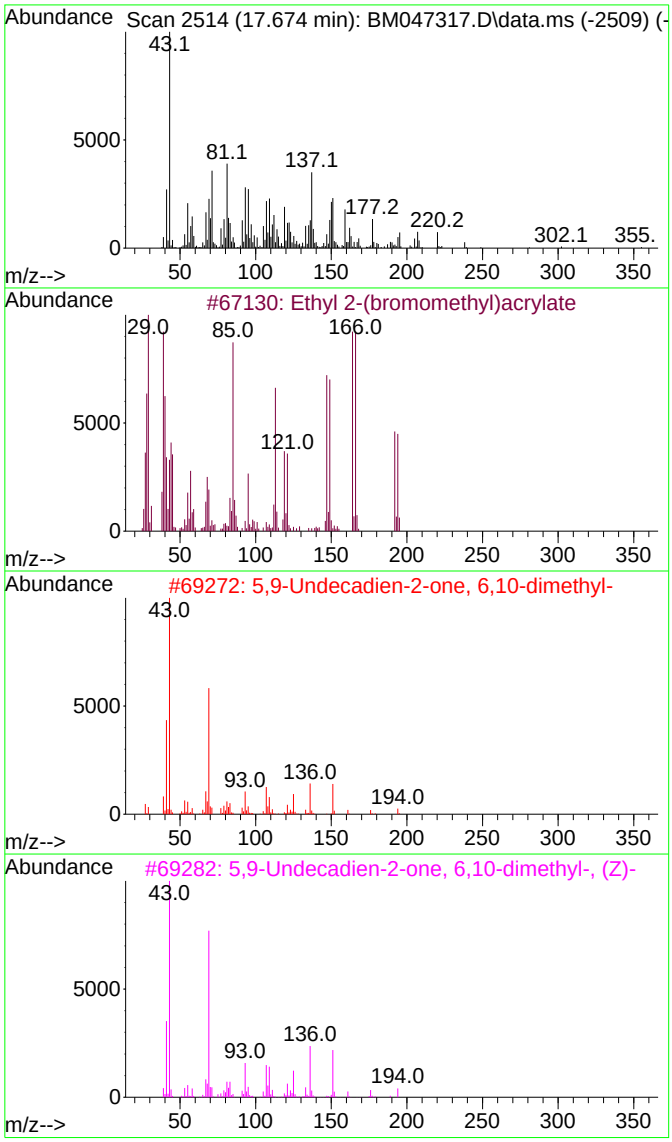
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

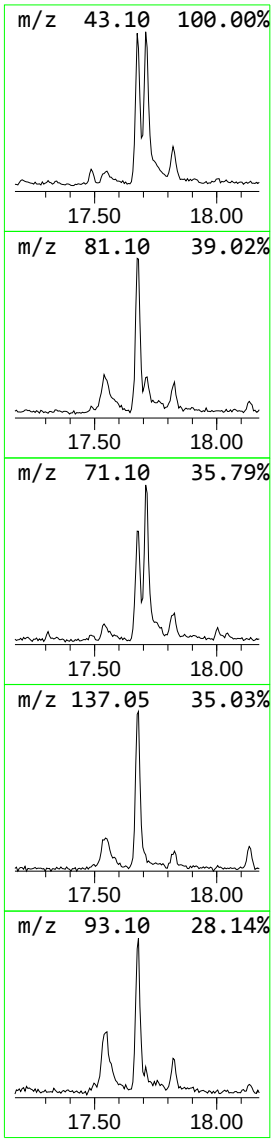
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethyl 2-(bromomethyl)acrylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.674	3.21 ng	557574	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 2-(bromomethyl)acrylate	192	C6H9BrO2	017435-72-2	91
2	5,9-Undecadien-2-one, 6,10-dimet...	194	C13H22O	000689-67-8	30
3	5,9-Undecadien-2-one, 6,10-dimet...	194	C13H22O	003879-26-3	27
4	Widdrol hydroxyether	238	C15H26O2	029620-91-5	22
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	152	C10H16O	001195-92-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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

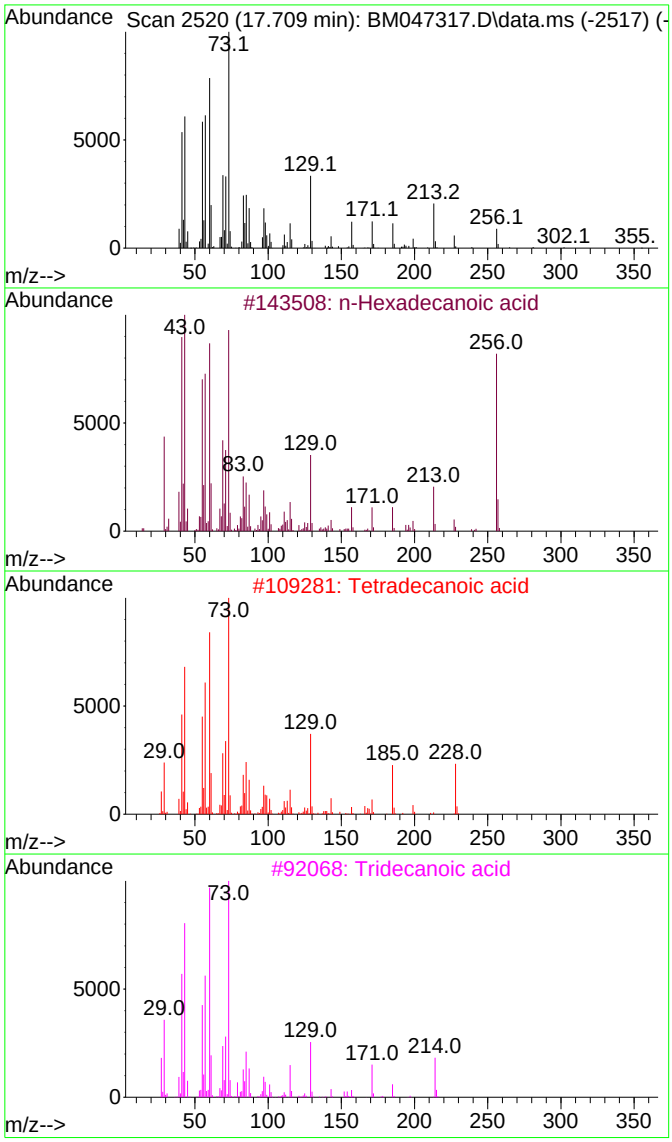
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

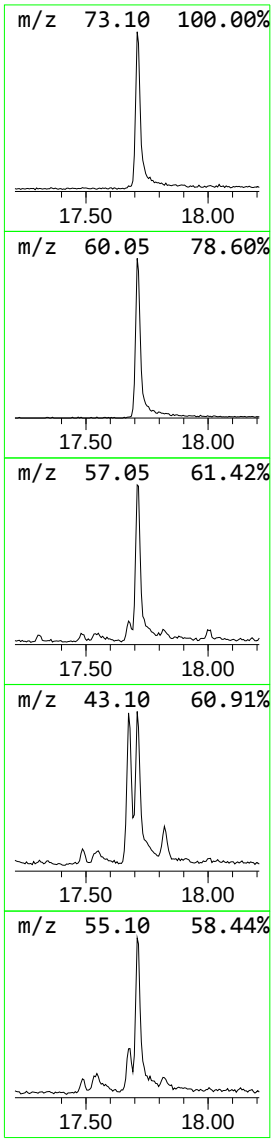
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	3.50 ng	607044	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

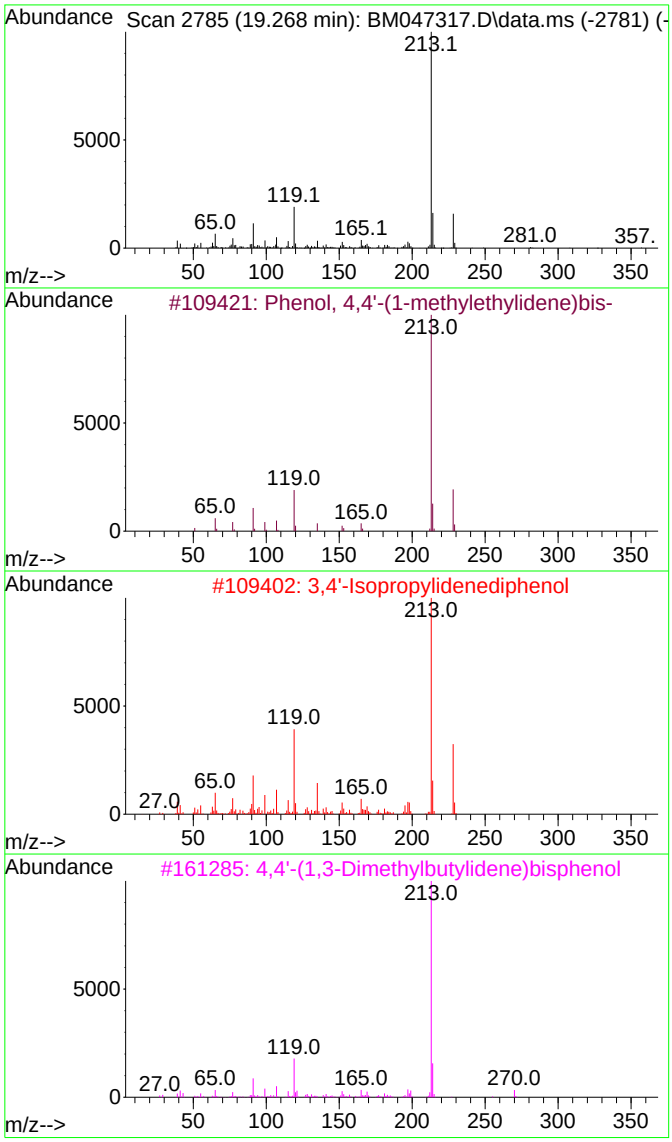
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

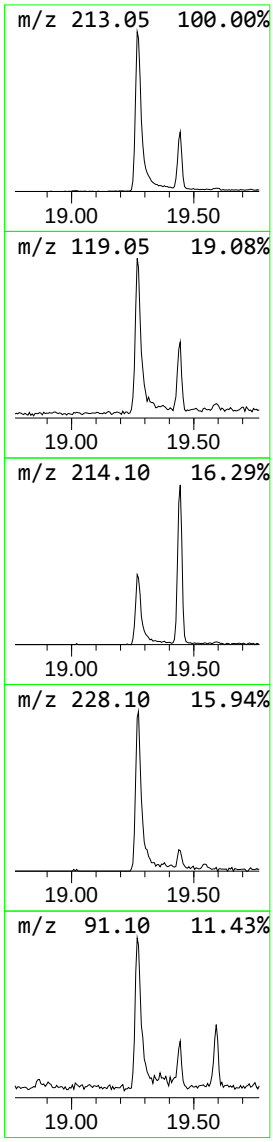
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	2.74 ng	477858	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	78
3	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	72
4	Stannane, chlorotriethyl-	242	C6H15ClSn	000994-31-0	59
5	Diphenolic acid	286	C17H18O4	000126-00-1	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

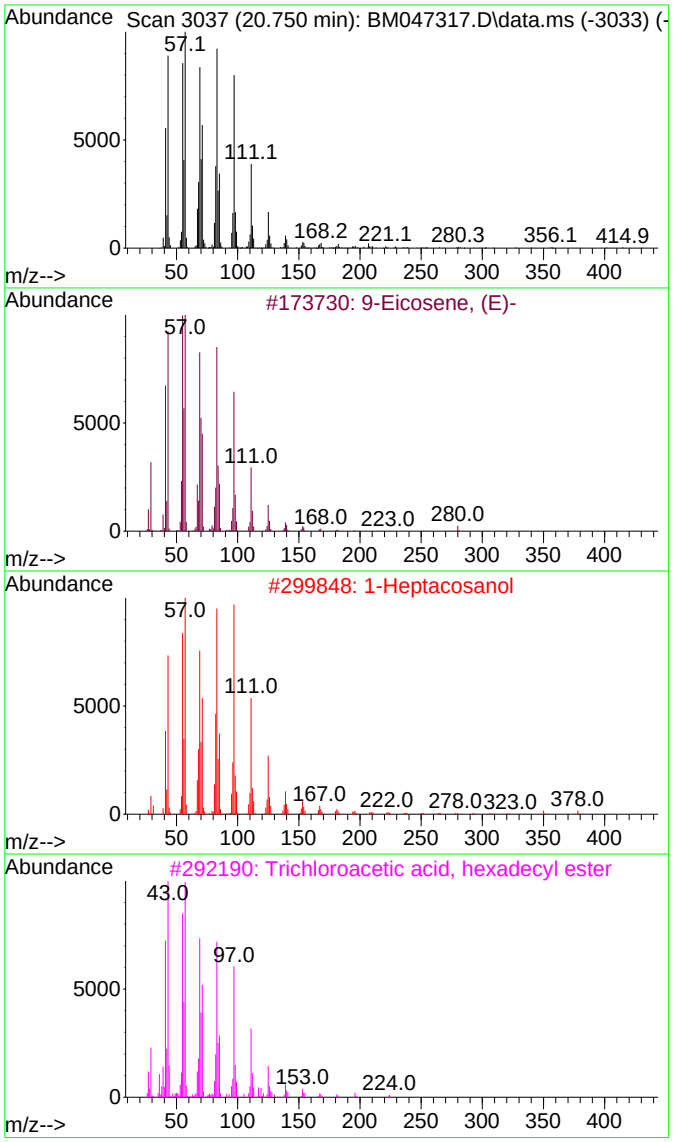
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

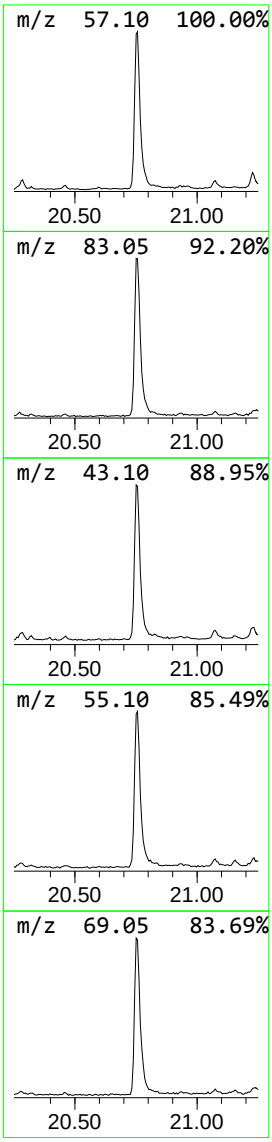
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 9-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	8.39 ng	1463010	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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

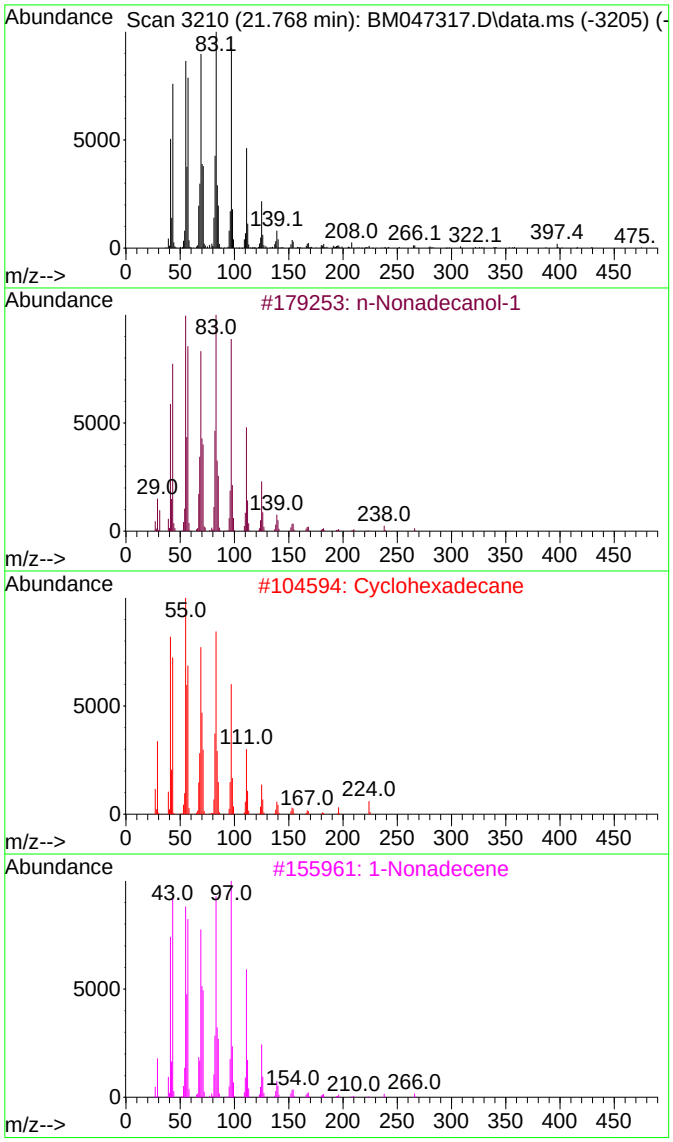
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

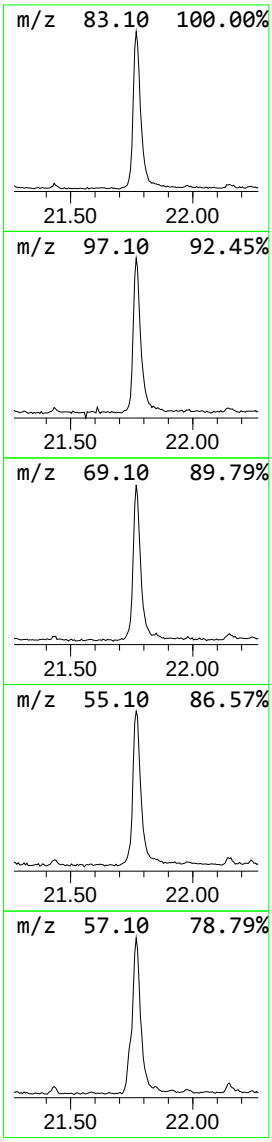
****

Peak Number 11 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.768	8.36 ng	1458430	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Cyclohexadecane	224	C16H32	000295-65-8	93
3	1-Nonadecene	266	C19H38	018435-45-5	93
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047317.D
Acq On : 22 Aug 2024 15:10
Operator : RC/JU
Sample : P3671-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0.5-1-081924

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	3.257	4.5	ng	325526	1	7.351	1432650	20.0
2-Pentanone, 4-...	4.563	4.0	ng	286553	1	7.351	1432650	20.0
Eucalyptol	7.651	6.4	ng	460135	1	7.351	1432650	20.0
1-Phenoxypropan...	10.874	3.5	ng	337333	2	10.104	1945560	20.0
Naphthalene, 1,...	14.268	2.7	ng	366517	3	14.010	2688730	20.0
(3S,3aS,6R,7R,9...	17.539	2.4	ng	418387	4	16.774	3471110	20.0
Ethyl 2-(bromom...	17.674	3.2	ng	557574	4	16.774	3471110	20.0
n-Hexadecanoic ...	17.709	3.5	ng	607044	4	16.774	3471110	20.0
Phenol, 4,4'-(1...	19.268	2.7	ng	477858	5	21.015	3487600	20.0
9-Eicosene, (E)-	20.750	8.4	ng	1463010	5	21.015	3487600	20.0
n-Nonadecanol-1	21.768	8.4	ng	1458430	5	21.015	3487600	20.0