LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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: BM047315.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	60	63	78	rVB	111134	178440	3.35%	0.383%
2	4.563	278	285	293	rBV	160152	226705	4.26%	0.487%
3	5.010	355	361	374	rBV	2209210	3245632	60.96%	6.972%
4	6.569	615	626	644	rBV	2131987	3531712	66.33%	7.587%
5	7.351	752	759	769	rBV	1030616	1558564	29.27%	3.348%
6	7.651	803	810	817	rVB	310282	459464	8.63%	0.987%
7	8.498	943	954	969	rBV	1460732	2465292	46.30%	5.296%
8	9.086	1049	1054	1067	rVB2	49156	96521	1.81%	0.207%
9	10.104	1220	1227	1239	rBV	1267748	2089172	39.24%	4.488%
10	10.686	1318	1326	1336	rVB6	21241	53994	1.01%	0.116%
11	10.875	1350	1358	1365	rBV	87348	203110	3.81%	0.436%
12	12.616	1647	1654	1673	rBV	2565729	3983946	74.83%	8.558%
13	14.010	1884	1891	1903	rBV	1856686	2903176	54.53%	6.237%
14	14.268	1927	1935	1941	rBV3	130773	250955	4.71%	0.539%
15	15.415	2122	2130	2135	rBV9	20341	54159	1.02%	0.116%
16	15.521	2142	2148	2160	rVV	2436247	3646211	68.48%	7.833%
17	15.762	2184	2189	2194	rBV	67399	93413	1.75%	0.201%
18	16.345	2283	2288	2293	rBV4	49474	89766	1.69%	0.193%
19	16.439	2300	2304	2311	rBV2	43090	63787	1.20%	0.137%
20	16.774	2349	2361	2371	rBV	2351174	3705022	69.59%	7.959%
21	16.898	2378	2382	2392	rVB6	32368	63286	1.19%	0.136%
22	16.986	2392	2397	2407	rBV9	108455	267282	5.02%	0.574%
23	17.486	2479	2482	2486	rBV4	31768	56798	1.07%	0.122%
24	17.545	2486	2492	2508	rVB3	140119	399324	7.50%	0.858%
25	17.680	2509	2515	2517	rBV	384008	532740	10.01%	1.144%
26	17.709	2517	2520	2527	rVB	355052	501379	9.42%	1.077%
27	17.821	2535	2539	2549	rVB5	84351	146521	2.75%	0.315%
28	18.639	2674	2678	2684	rBV4	44572	74697	1.40%	0.160%
29	18.856	2710	2715	2719	rBV	78873	128943	2.42%	0.277%
30	19.015	2738	2742	2750	rBV	142921	223771	4.20%	0.481%
31	19.268	2781	2785	2797	rVV	404221	743119	13.96%	1.596%
32	19.374	2799	2803	2806	rVV3	41845	61567	1.16%	0.132%
33	19.445	2806	2815	2826	rVB	3961412	5324300	100.00%	11.438%
34	19.592	2837	2840	2846	rVB	83546	100917	1.90%	0.217%
35	19.892	2887	2891	2899	rBV3	57273	99129	1.86%	0.213%
36	20.756	3033	3038	3053	rBV	598564	1081442	20.31%	2.323%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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	21.015	3077	3082	3089	rBV2	2620005	3550936	66.69%	7.628%
38	21.768	3206	3210	3221	rVB2	450938	991232	18.62%	2.129%
39	23.709	3532	3540	3552	rVB	1395775	3304776	62.07%	7.099%

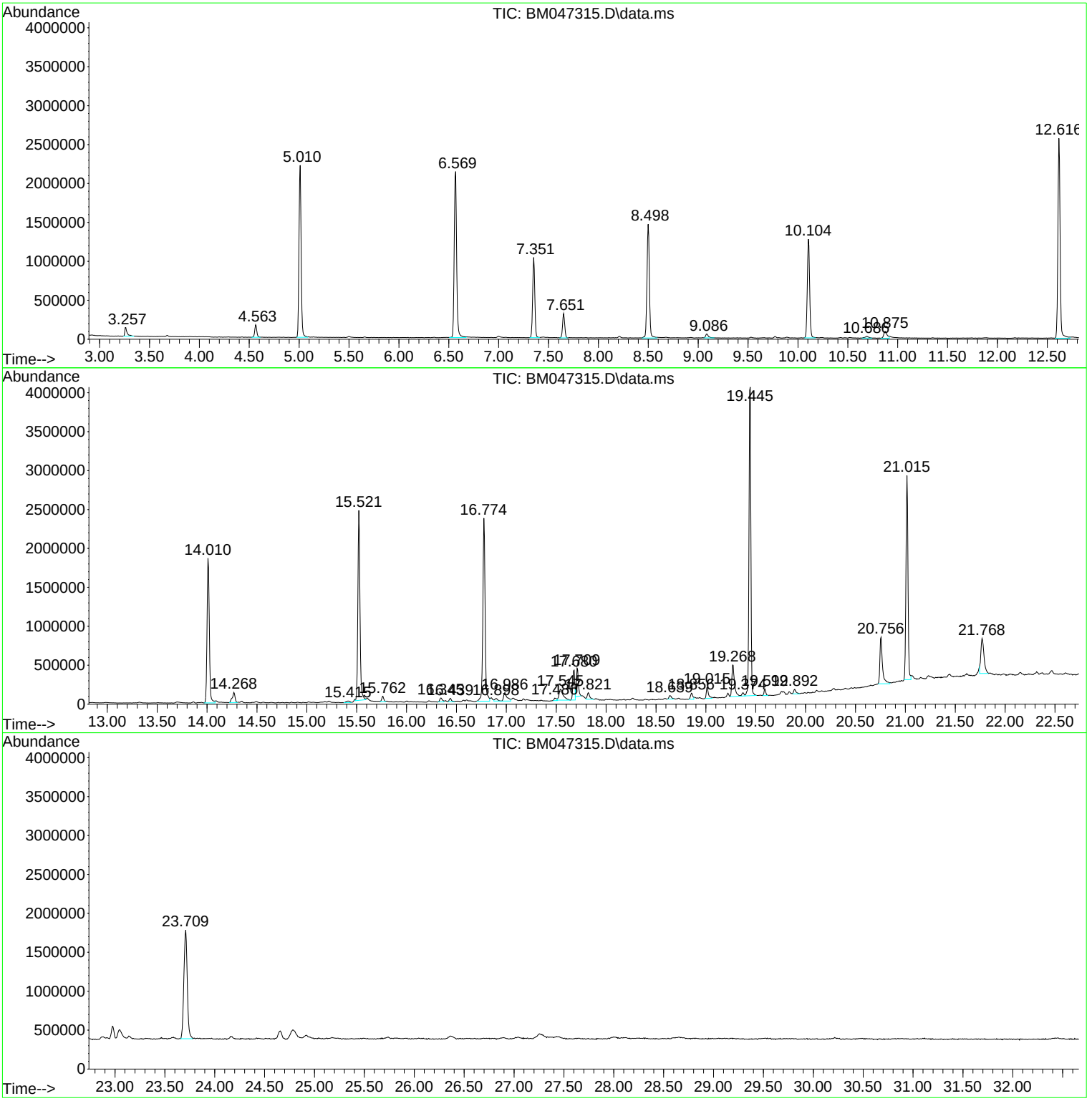
Sum of corrected areas: 46551200

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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 : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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

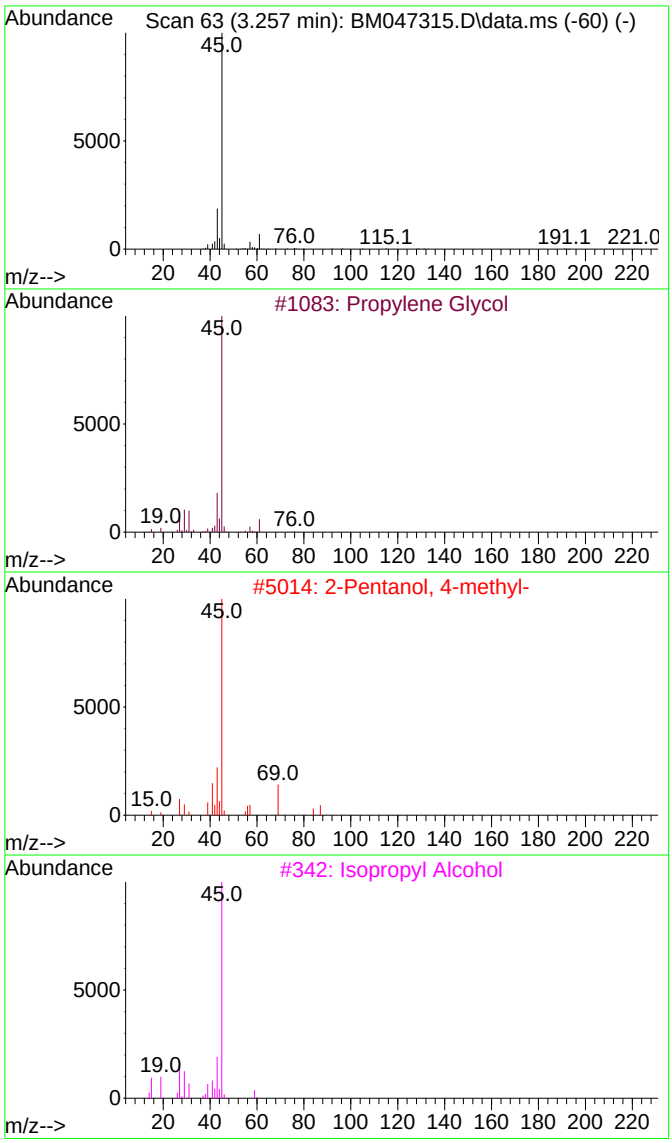
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

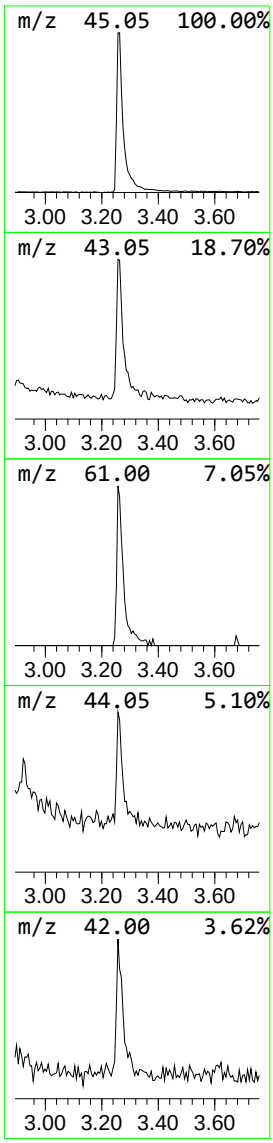
****

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	2.29 ng	178440	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	39
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	2-Hexanol	102	C6H14O	000626-93-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

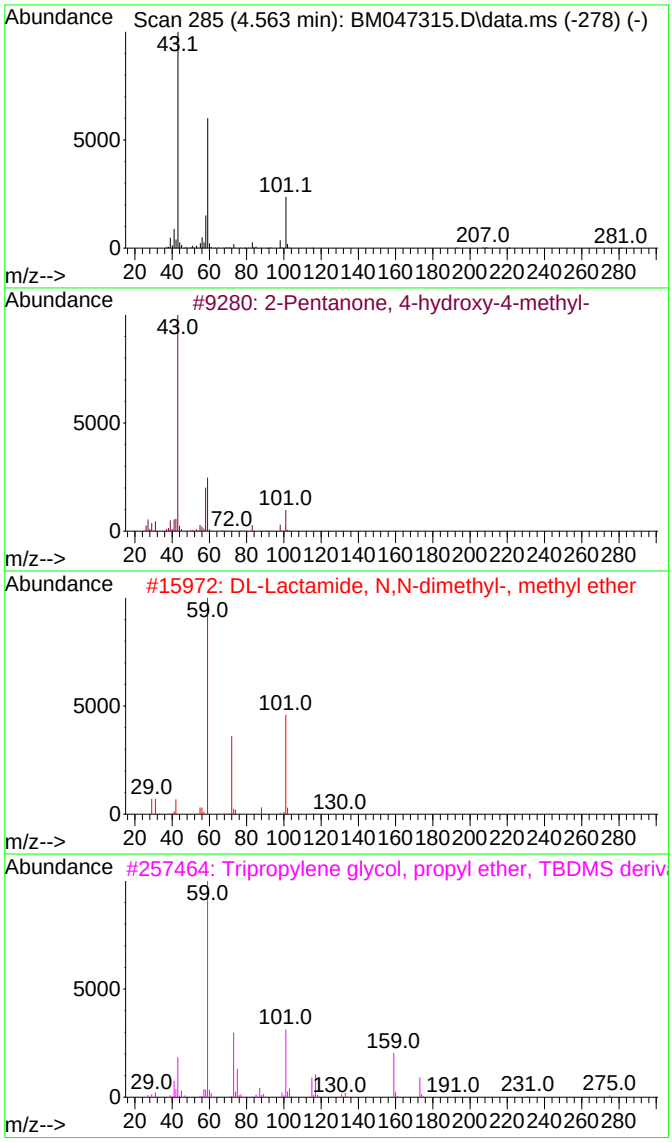
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

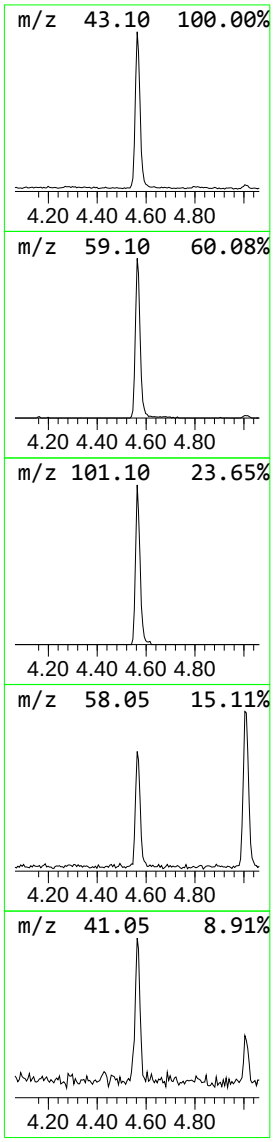
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	2.91 ng	226705	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	64
2	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	28
3	Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	28
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	Tetraglyme	222	C10H22O5	000143-24-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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

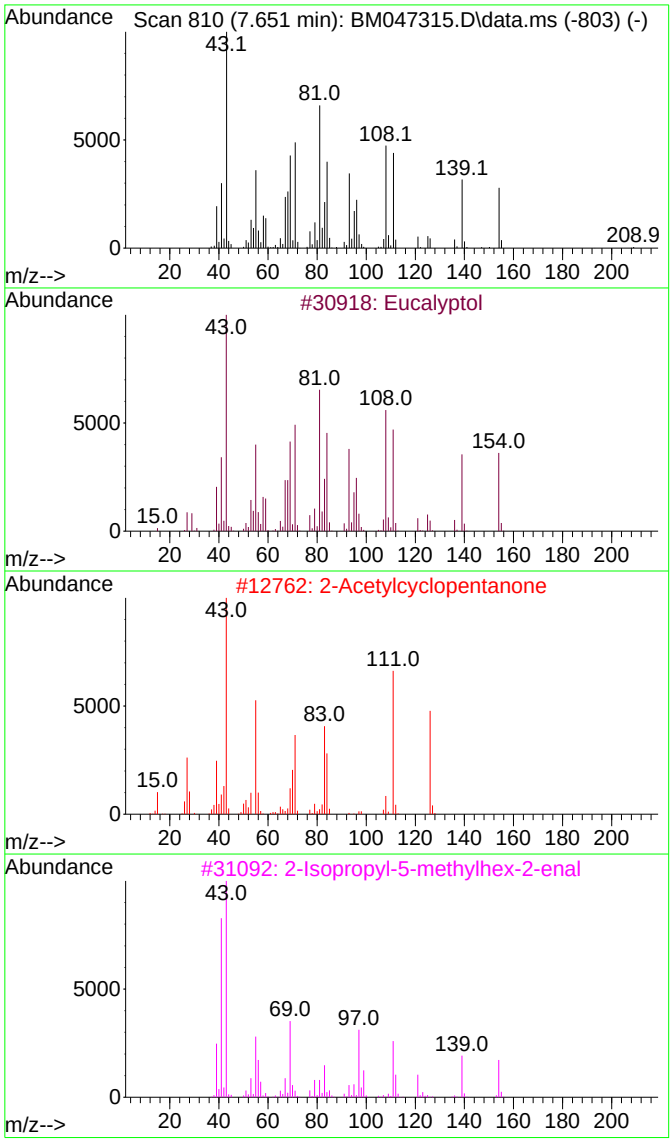
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

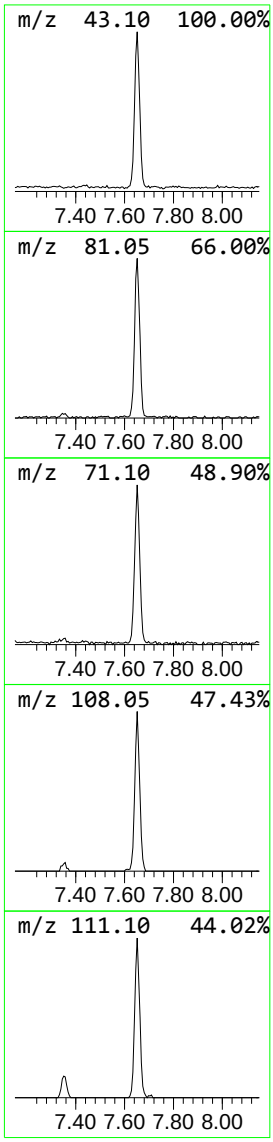
****

Peak Number 3 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	5.90 ng	459464	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
3	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
4	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

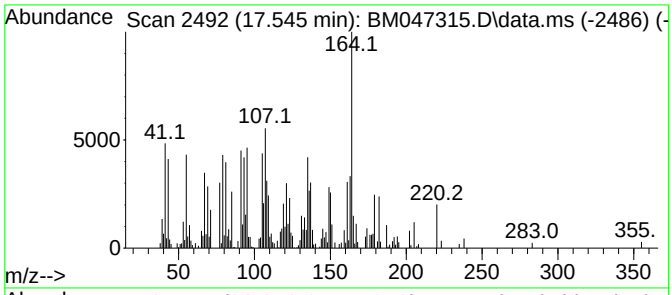
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

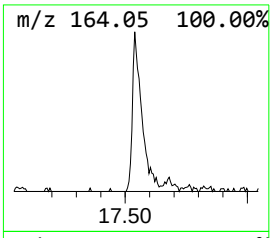
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

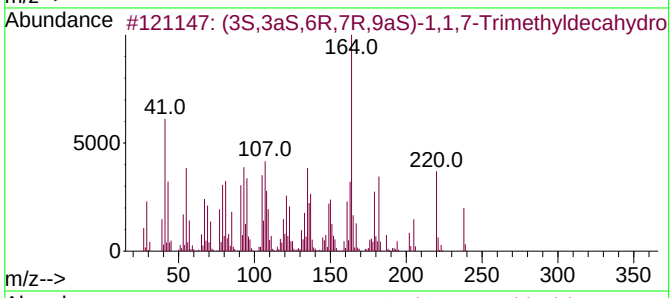
****
Peak Number 4 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 9

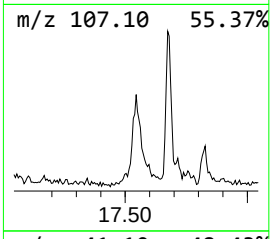
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.545	2.16 ng	399324	Phenanthrene-d10	16.774

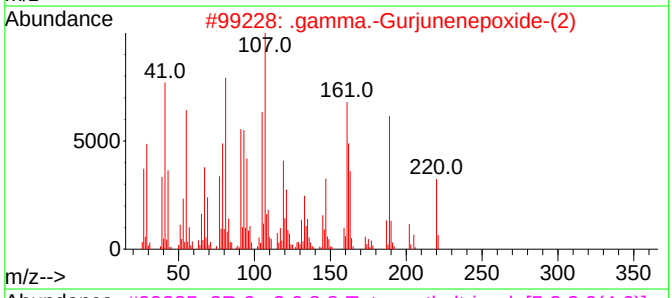
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	99
2	.gamma.-Gurjunenepoxide-(2)	220	C15H24O	184705-51-9	47
3	2R,6s-2,6,8,8-Tetramethyltricycl...	220	C15H24O	1000140-21-3	43
4	Benzene, 1-(allyloxy)-3-methoxy-	164	C10H12O2	037592-19-1	38
5	1-Benzoxepin-3-ol, 2,3,4,5-tetra...	164	C10H12O2	038824-30-5	30

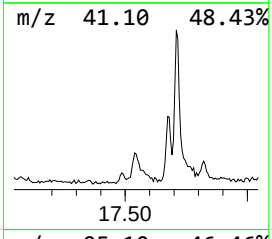


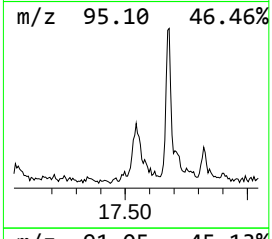


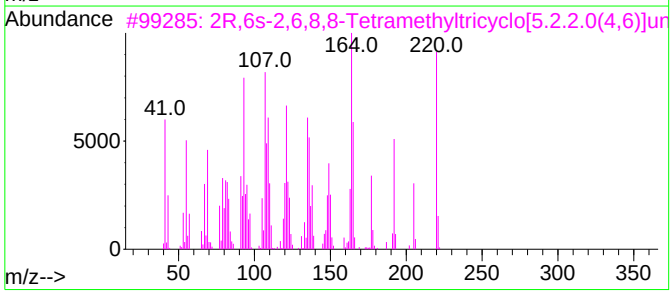


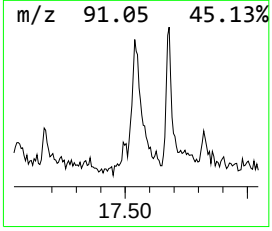












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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

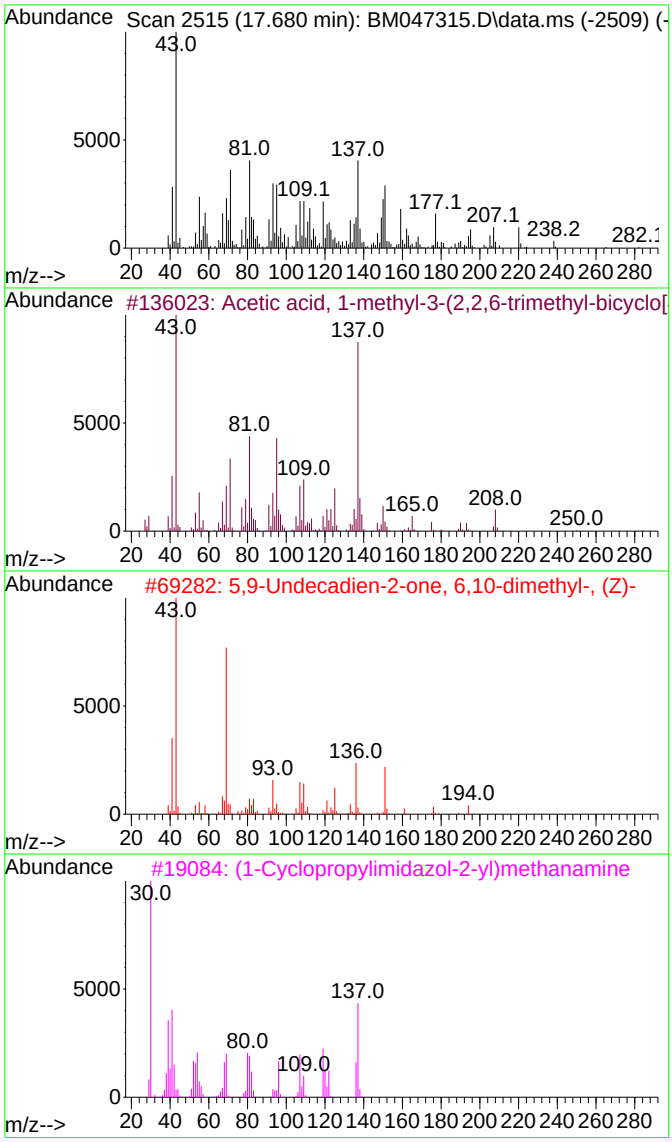
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

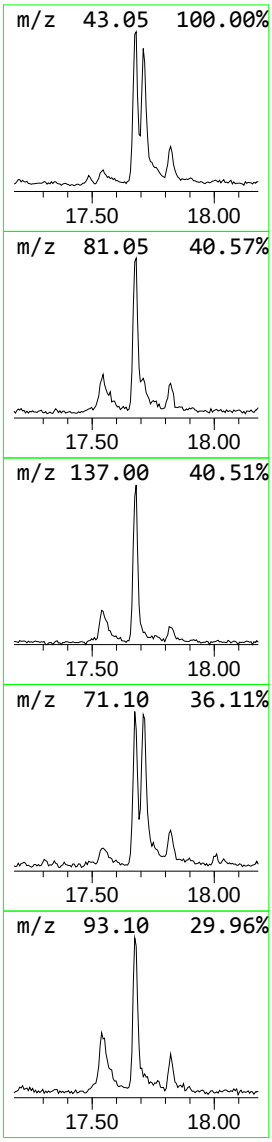
****

Peak Number 5 unknown17.680 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.680	2.88 ng	532740	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1-methyl-3-(2,2,6-t...	250	C16H26O2	1010192-25-5	35
2	5,9-Undecadien-2-one, 6,10-dimet...	194	C13H22O	003879-26-3	22
3	(1-Cyclopropylimidazol-2-yl)meth...	137	C7H11N3	1000444-19-0	22
4	7,11-Epoxymegastigma-5(6)-en-9-one	208	C13H20O2	064243-62-5	12
5	7-Hydroxyfarnesen	220	C15H24O	1000374-20-4	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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

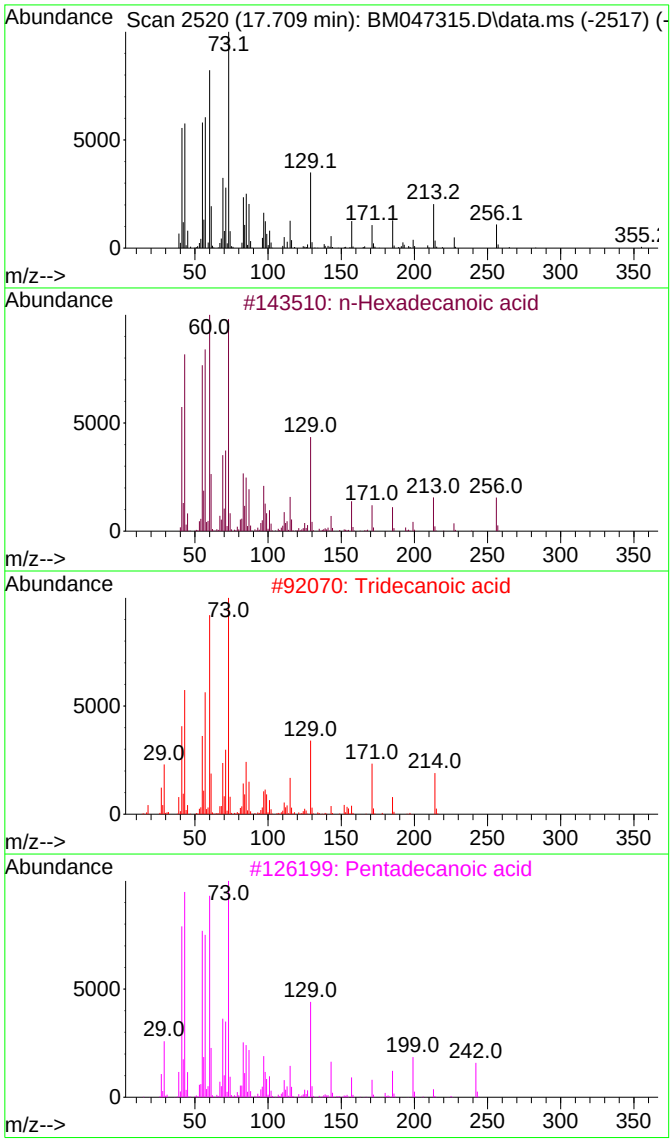
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

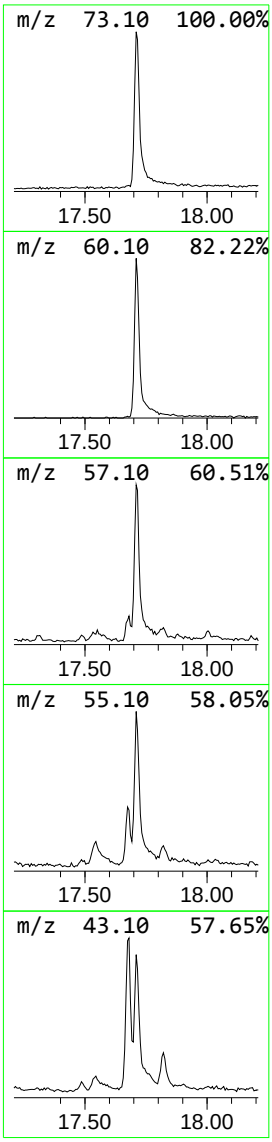
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	2.71 ng	501379	Phenanthrene-d10	16.774

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

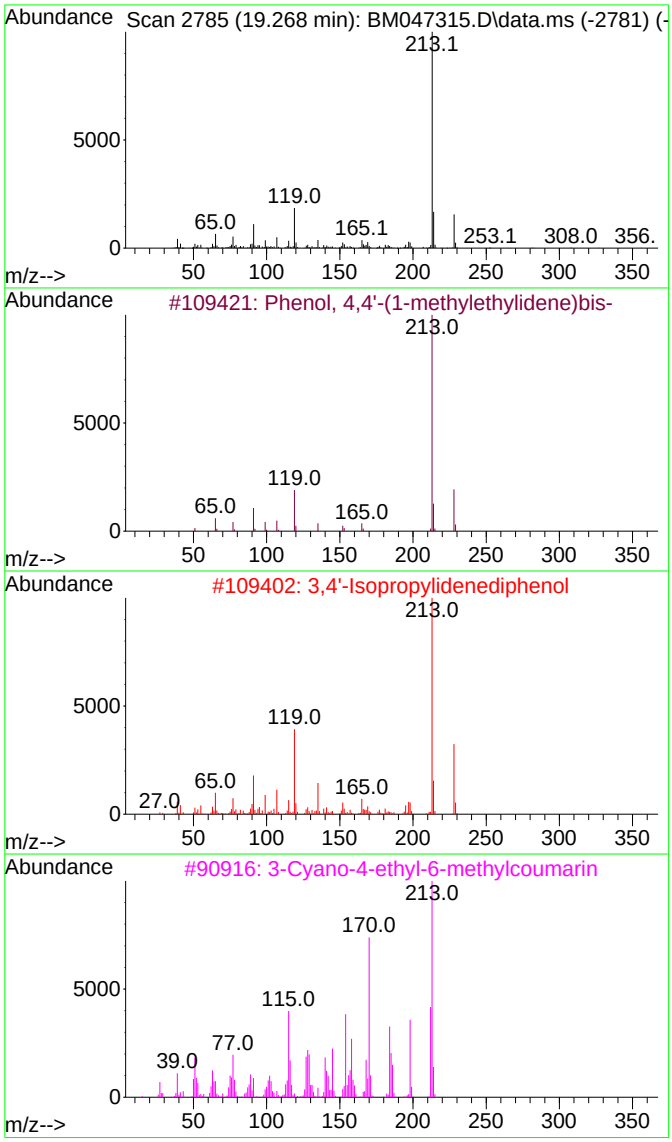
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

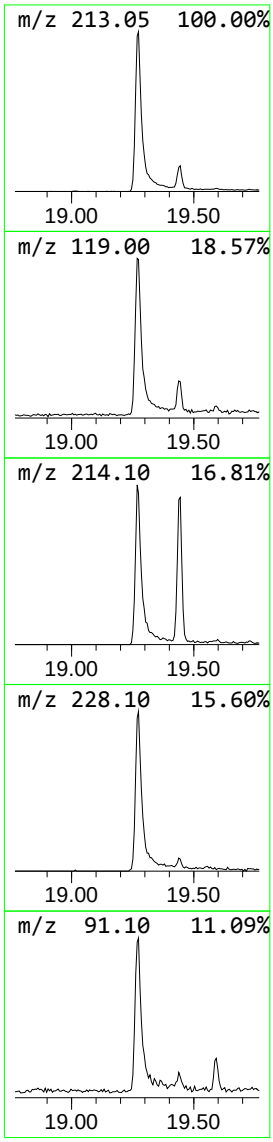
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	4.19 ng	743119	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	60
3	3-Cyano-4-ethyl-6-methylcoumarin	213	C13H11NO2	025937-11-5	53
4	3-Chloro-N,N-diethyl-4-nitroaniline	228	C10H13ClN2O2	1010110-36-0	53
5	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

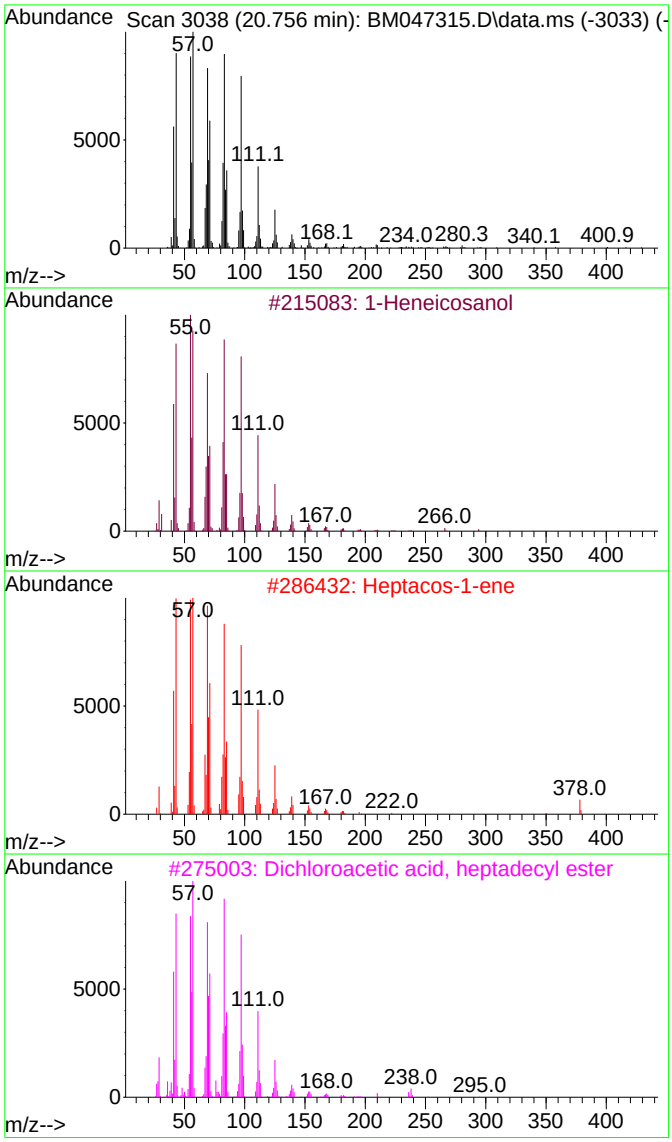
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

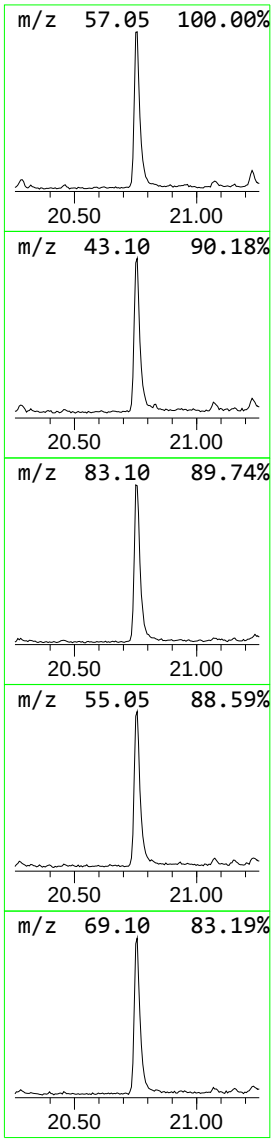
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	6.09 ng	1081440	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Heptacos-1-ene	378	C27H54	015306-27-1	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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

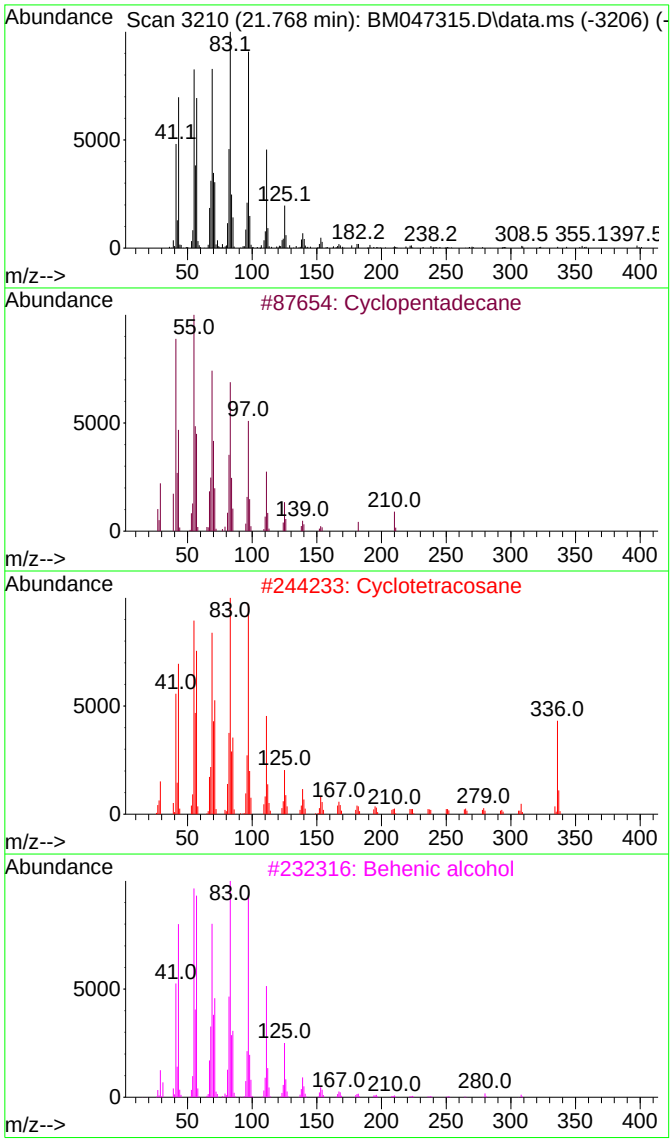
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

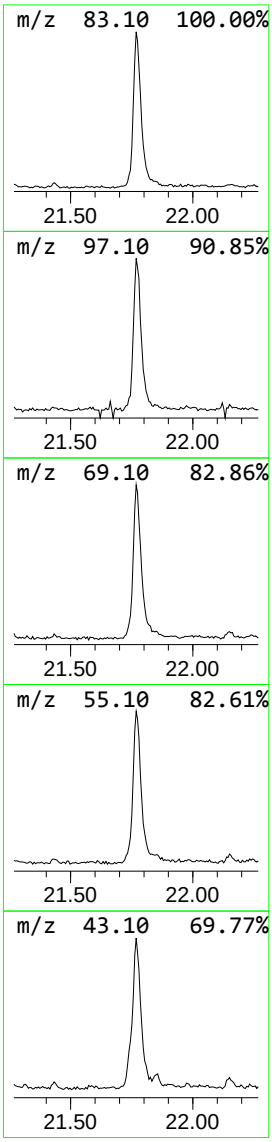
****

Peak Number 9 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.768	5.58 ng	991232	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	91
2	Cyclotetracosane	336	C24H48	000297-03-0	90
3	Behenic alcohol	326	C22H46O	000661-19-8	89
4	1-Octadecanol	270	C18H38O	000112-92-5	76
5	Octacosanol	410	C28H58O	000557-61-9	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047315.D
Acq On : 22 Aug 2024 13:51
Operator : RC/JU
Sample : P3671-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-928-KI-SO-0-0.5-081924

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	2.3	ng	178440	1	7.351	1558560	20.0
2-Pentanone, 4-...	4.563	2.9	ng	226705	1	7.351	1558560	20.0
Eucalyptol	7.651	5.9	ng	459464	1	7.351	1558560	20.0
(3S,3aS,6R,7R,9...	17.545	2.2	ng	399324	4	16.774	3705020	20.0
unknown17.680	17.680	2.9	ng	532740	4	16.774	3705020	20.0
n-Hexadecanoic ...	17.709	2.7	ng	501379	4	16.774	3705020	20.0
Phenol, 4,4'-(1...	19.268	4.2	ng	743119	5	21.015	3550940	20.0
1-Heneicosanol	20.756	6.1	ng	1081440	5	21.015	3550940	20.0
Cyclopentadecane	21.768	5.6	ng	991232	5	21.015	3550940	20.0