LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

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-BM052323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	302	307	314	rBV	433487	580909	5.39%	0.647%
2	5.563	380	387	397	rBV	5095652	7073447	65.58%	7.873%
3	6.693	573	579	587	rVB	370482	549341	5.09%	0.611%
4	7.169	650	660	674	rBV	4692324	7118590	66.00%	7.924%
5	8.016	797	804	812	rBV	1450143	2193146	20.33%	2.441%
6	9.181	994	1002	1013	rBV	2664441	4255405	39.45%	4.737%
7	10.834	1275	1283	1290	rBV	1817920	2940967	27.27%	3.274%
8	13.280	1692	1699	1706	rBV	6587993	9182470	85.13%	10.221%
9	13.539	1737	1743	1750	rBV	182163	256395	2.38%	0.285%
10	13.927	1804	1809	1813	rBV2	74497	112278	1.04%	0.125%
11	13.980	1813	1818	1825	rVV2	931379	1320825	12.25%	1.470%
12	14.069	1827	1833	1839	rVV	182408	261024	2.42%	0.291%
13	14.369	1878	1884	1889	rBV	295126	424264	3.93%	0.472%
14	14.498	1897	1906	1910	rBV3	106440	196435	1.82%	0.219%
15	14.616	1917	1926	1929	rBV	4052218	5321899	49.34%	5.924%
16	14.651	1929	1932	1938	rVB	2286442	3128654	29.01%	3.482%
17	14.751	1946	1949	1959	rVB3	121143	234597	2.17%	0.261%
18	14.904	1969	1975	1981	rVB	331454	457561	4.24%	0.509%
19	14.980	1981	1988	1997	rBV3	192905	330808	3.07%	0.368%
20	16.004	2152	2162	2169	rBV	857650	1325281	12.29%	1.475%
21	16.133	2177	2184	2191	rVB	4873633	6665706	61.80%	7.419%
22	16.568	2253	2258	2262	rBV	108020	139147	1.29%	0.155%
23	17.392	2392	2398	2404	rBV	2384905	3238982	30.03%	3.605%
24	18.286	2544	2550	2559	rBV	572870	926625	8.59%	1.031%
25	18.362	2559	2563	2571	rVB	115074	193747	1.80%	0.216%
26	19.445	2743	2747	2752	rBV	138370	193276	1.79%	0.215%
27	19.556	2762	2766	2779	rBV	380596	683810	6.34%	0.761%
28	19.780	2800	2804	2806	rBV2	112455	167049	1.55%	0.186%
29	19.809	2806	2809	2823	rVB	212164	349322	3.24%	0.389%
30	20.009	2837	2843	2855	rBV	9481347	10786405	100.00%	12.006%
31	20.174	2868	2871	2876	rVB	119155	131208	1.22%	0.146%
32	20.321	2892	2896	2899	rBV3	101567	117631	1.09%	0.131%
33	20.962	3001	3005	3010	rBV	239608	268739	2.49%	0.299%
34	21.121	3027	3032	3042	rVB	6555115	7666025	71.07%	8.533%
35	21.274	3054	3058	3067	rBV	596744	791660	7.34%	0.881%
36	21.486	3090	3094	3100	rBV	300068	379003	3.51%	0.422%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

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-BM052323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.568	3102	3108	3112	rVV	2814255	3916349	36.31%	4.359%
38	21.609	3112	3115	3124	rVB	389313	540449	5.01%	0.602%
39	21.692	3126	3129	3132	rVV	149701	191131	1.77%	0.213%
40	21.727	3133	3135	3140	rVB	128101	152468	1.41%	0.170%
41	22.203	3213	3216	3223	rBV2	136009	194091	1.80%	0.216%
42	22.380	3241	3246	3250	rBV4	174401	433232	4.02%	0.482%
43	23.274	3394	3398	3402	rBV2	270335	467293	4.33%	0.520%
44	23.321	3403	3406	3414	rVB	231832	385350	3.57%	0.429%
45	24.021	3518	3525	3536	rVB	1829160	3597900	33.36%	4.005%

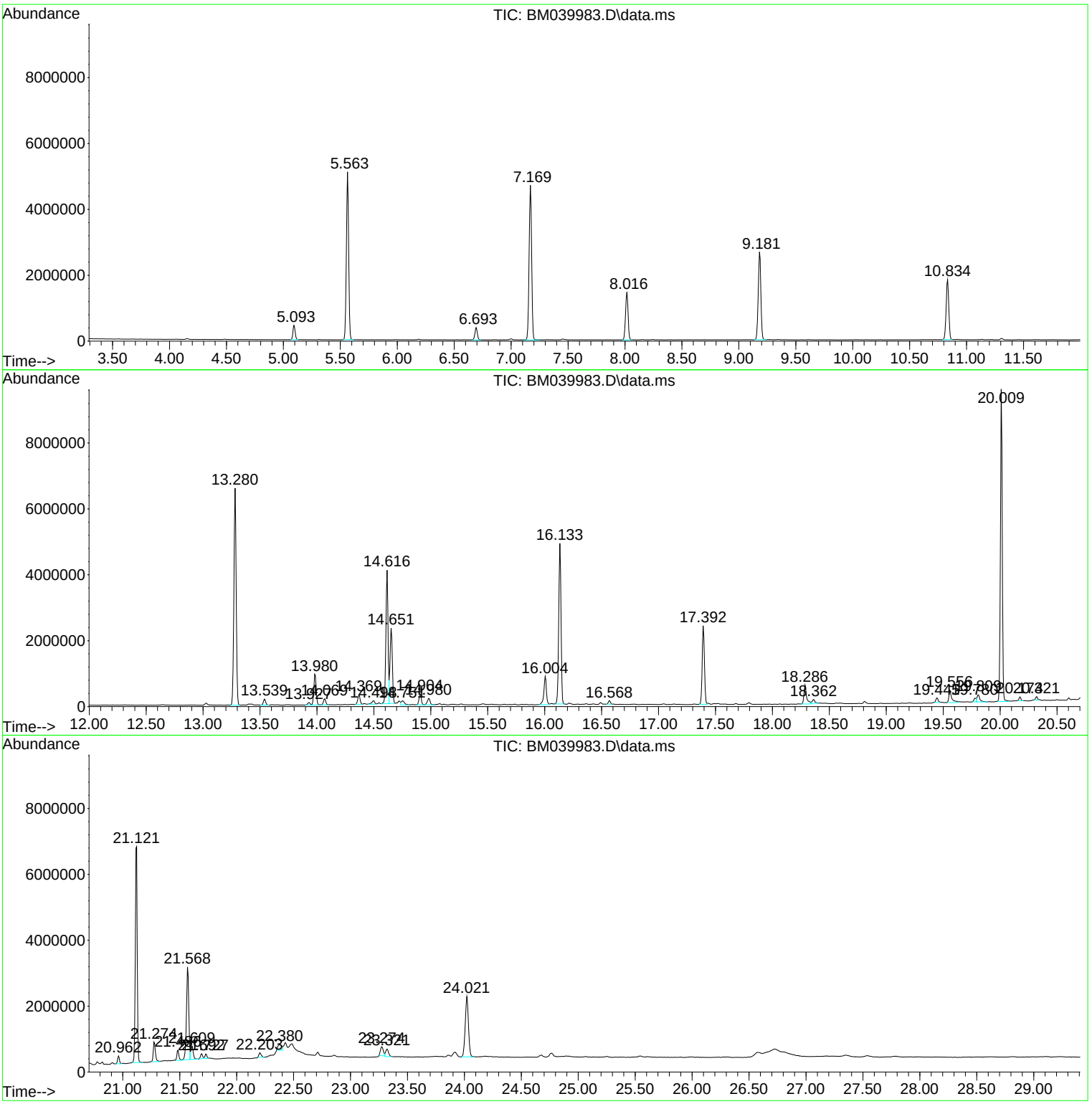
Sum of corrected areas: 89840894

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

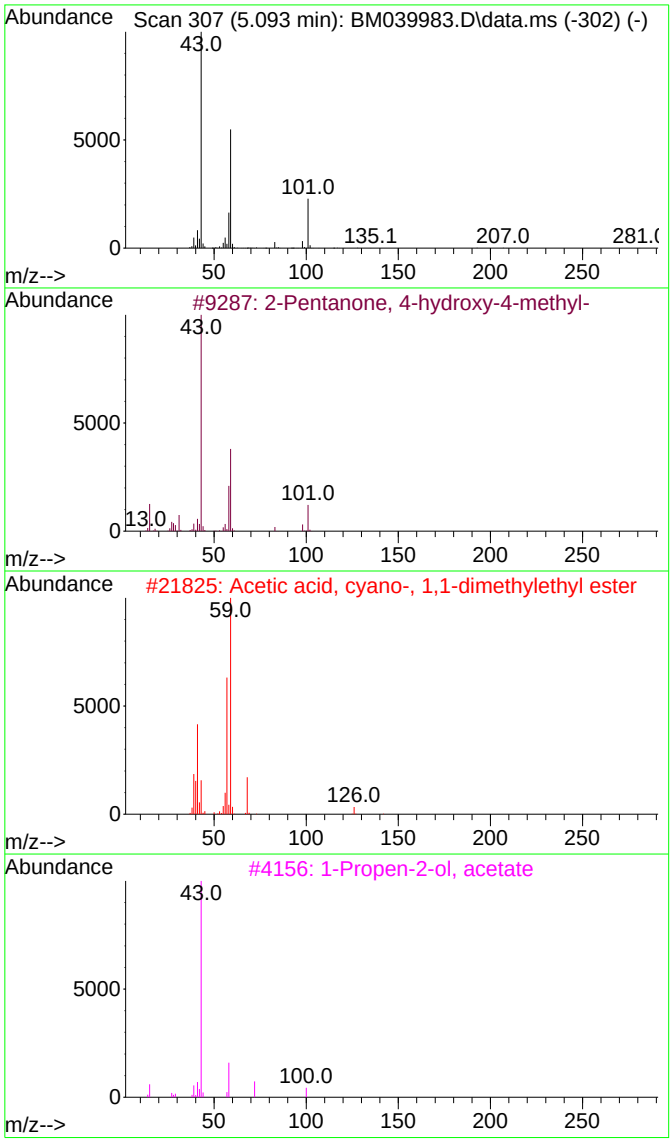
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

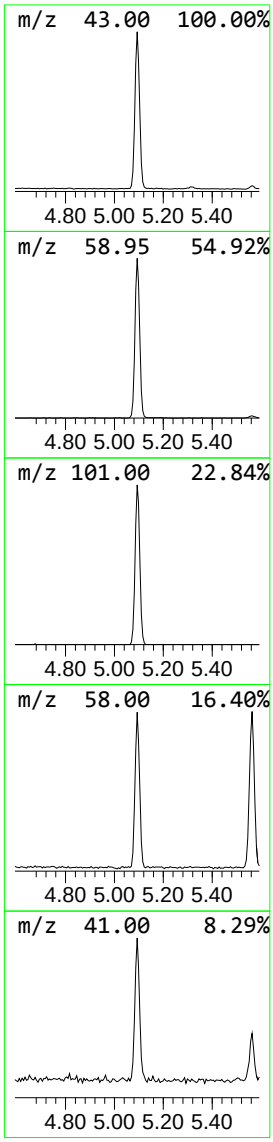
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	5.30 ng	580909	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

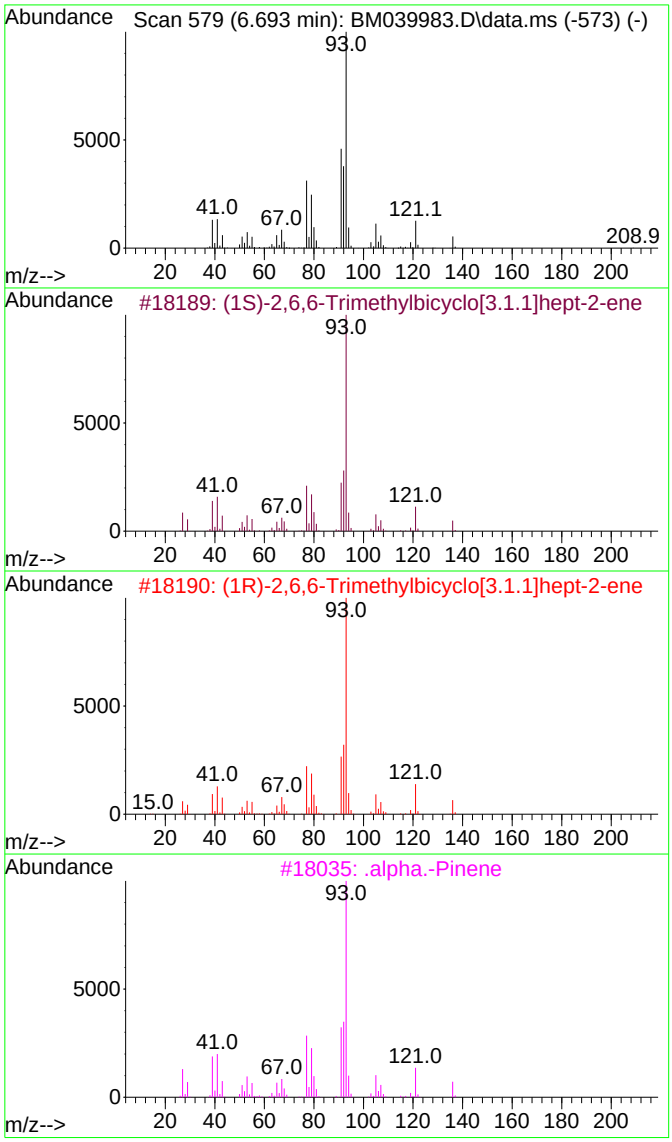
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

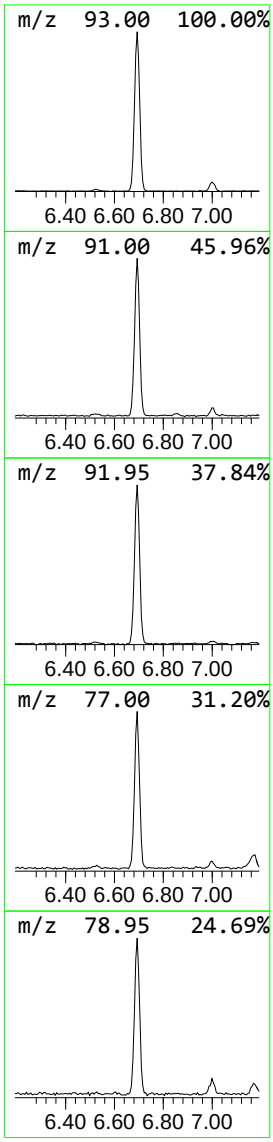
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.693	5.01 ng	549341	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	97
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	96
3	.alpha.-Pinene	136	C10H16	000080-56-8	96
4	3-Carene	136	C10H16	013466-78-9	91
5	(+)-3-Carene	136	C10H16	000498-15-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

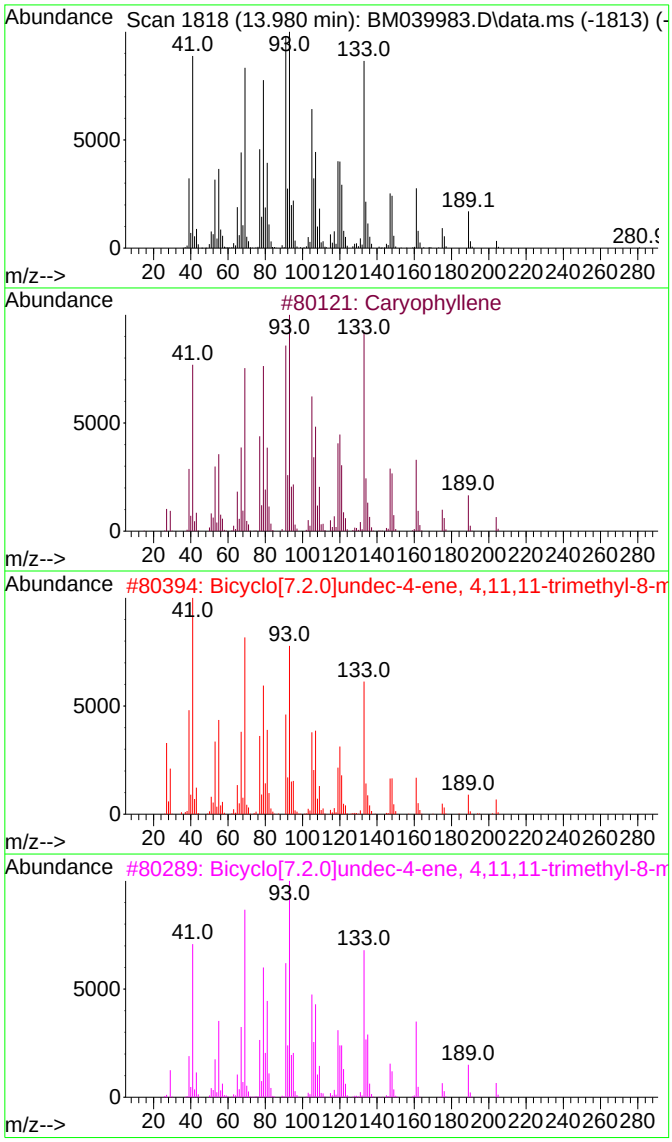
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

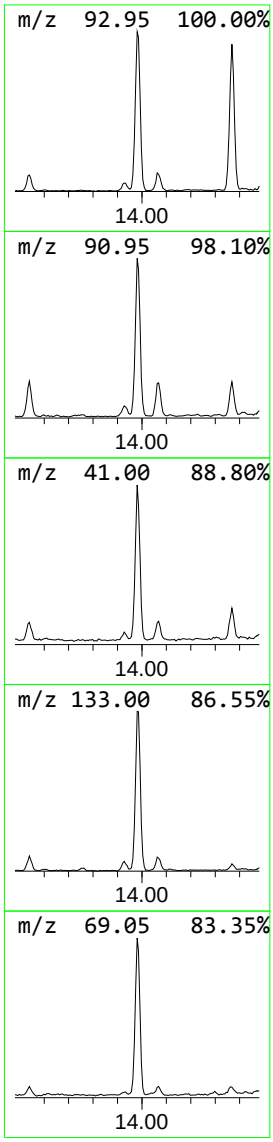
****

Peak Number 3 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	8.44 ng	1320830	Acenaphthene-d10	14.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	94
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	86
4	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	55
5	11,11-Dimethyl-spiro[2,9]dodeca-...	190	C14H22	1000062-28-4	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

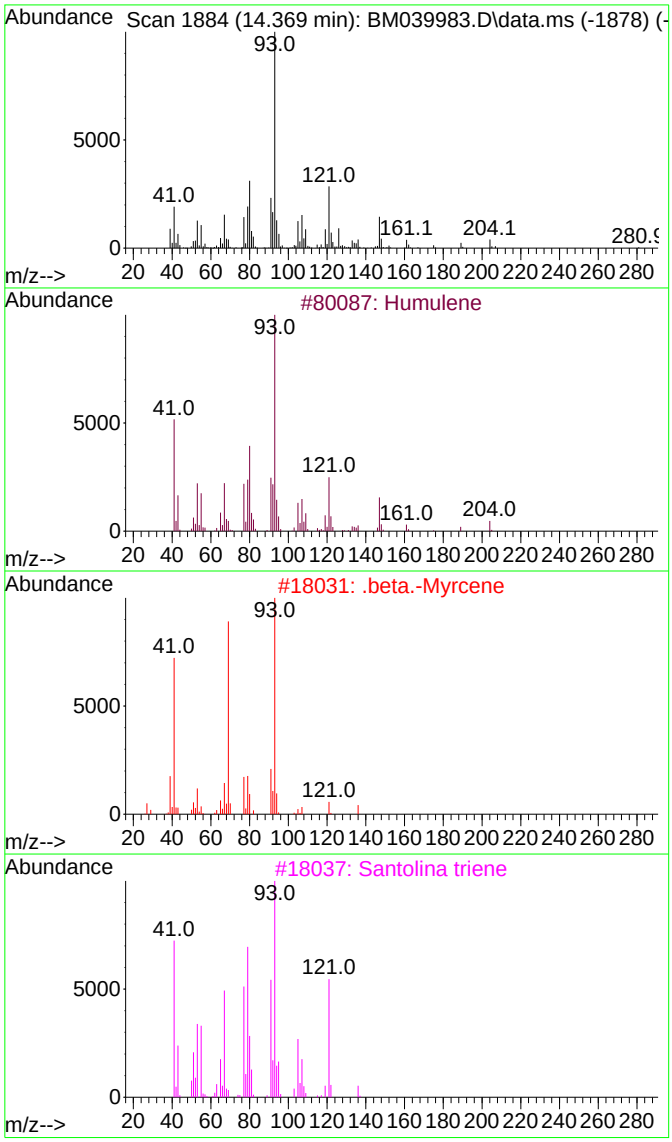
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

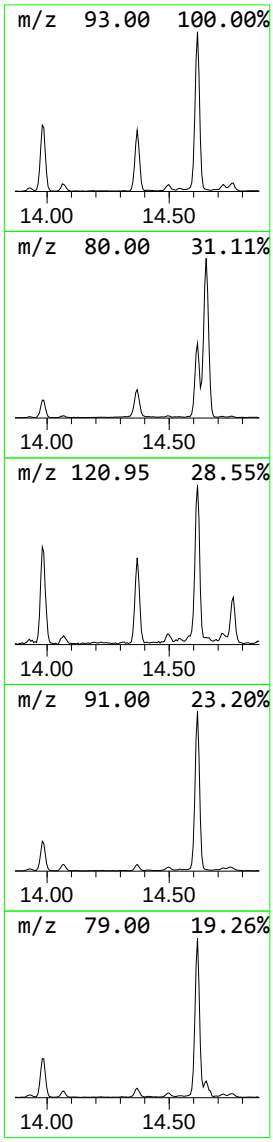
****

Peak Number 4 Humulene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.369	2.71 ng	424264	Acenaphthene-d10	14.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Humulene	204	C15H24	006753-98-6	97
2	.beta.-Myrcene	136	C10H16	000123-35-3	70
3	Santolina triene	136	C10H16	002153-66-4	58
4	1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	50
5	.gamma.-Terpinene	136	C10H16	000099-85-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

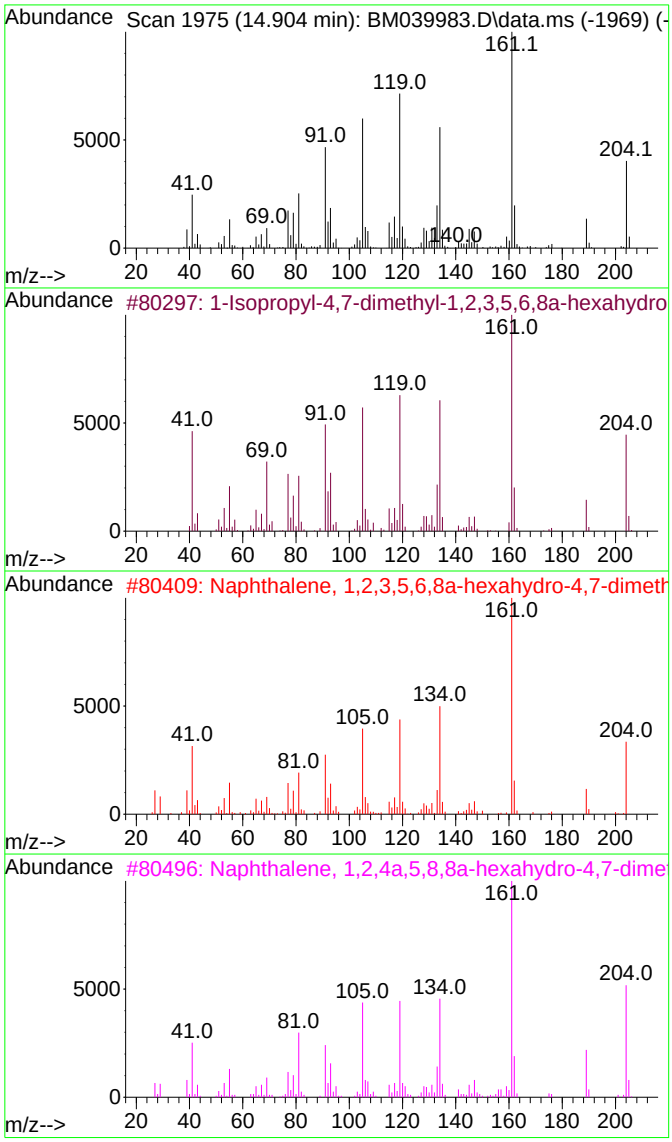
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

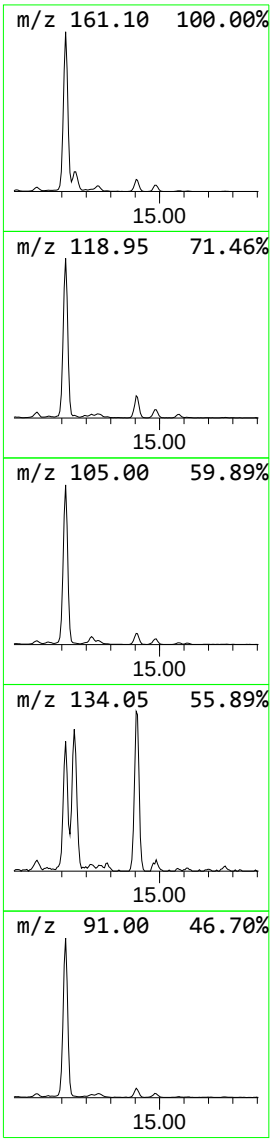
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Isopropyl-4,7-dimethyl-1,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.92 ng	457561	Acenaphthene-d10	14.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	98
2	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	97
3	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	93
4	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	89
5	.alpha.-Muurolene	204	C15H24	010208-80-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

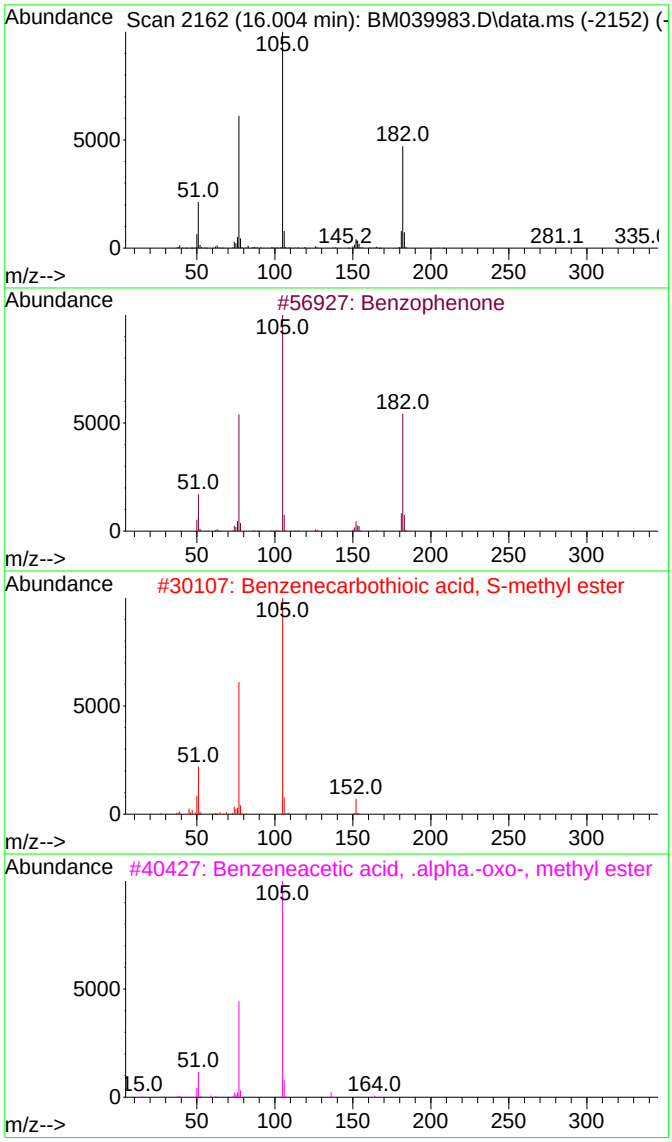
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

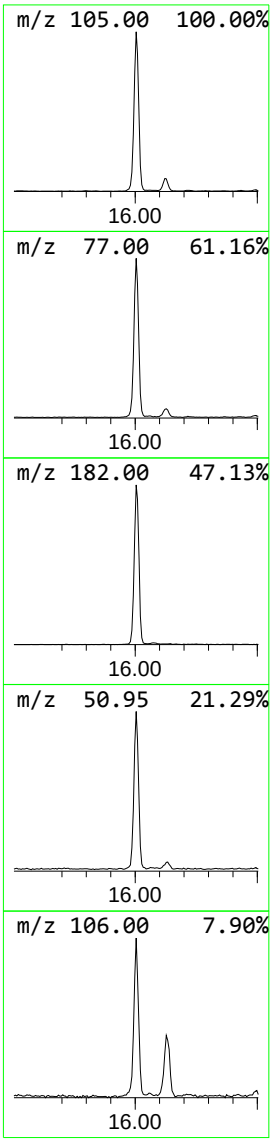
****

Peak Number 6 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	8.47 ng	1325280	Acenaphthene-d10	14.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

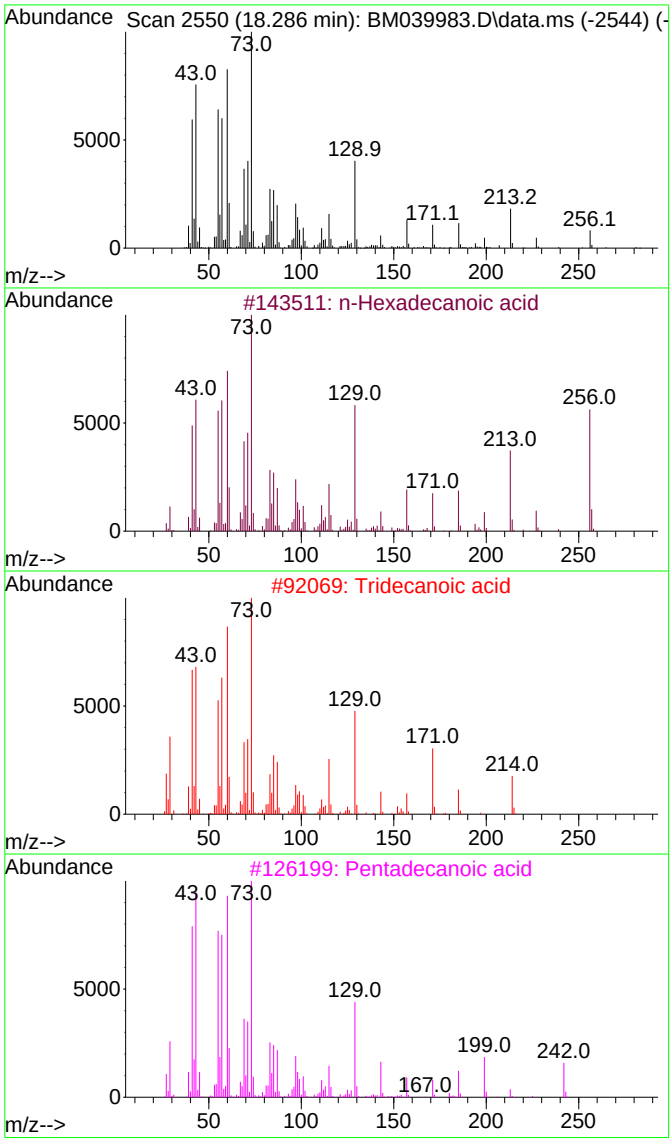
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

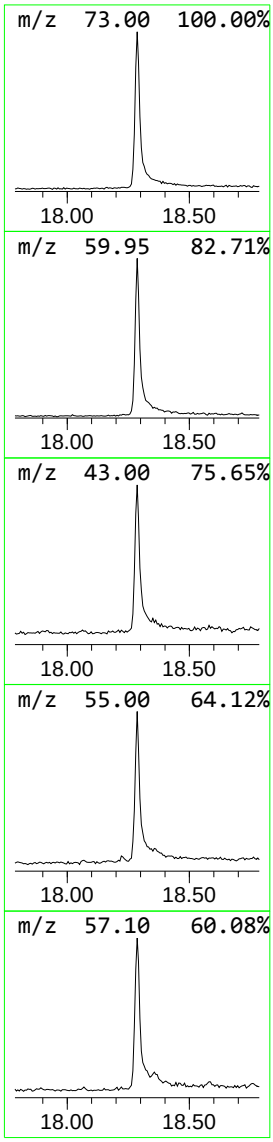
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	5.72 ng	926625	Phenanthrene-d10	17.392

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

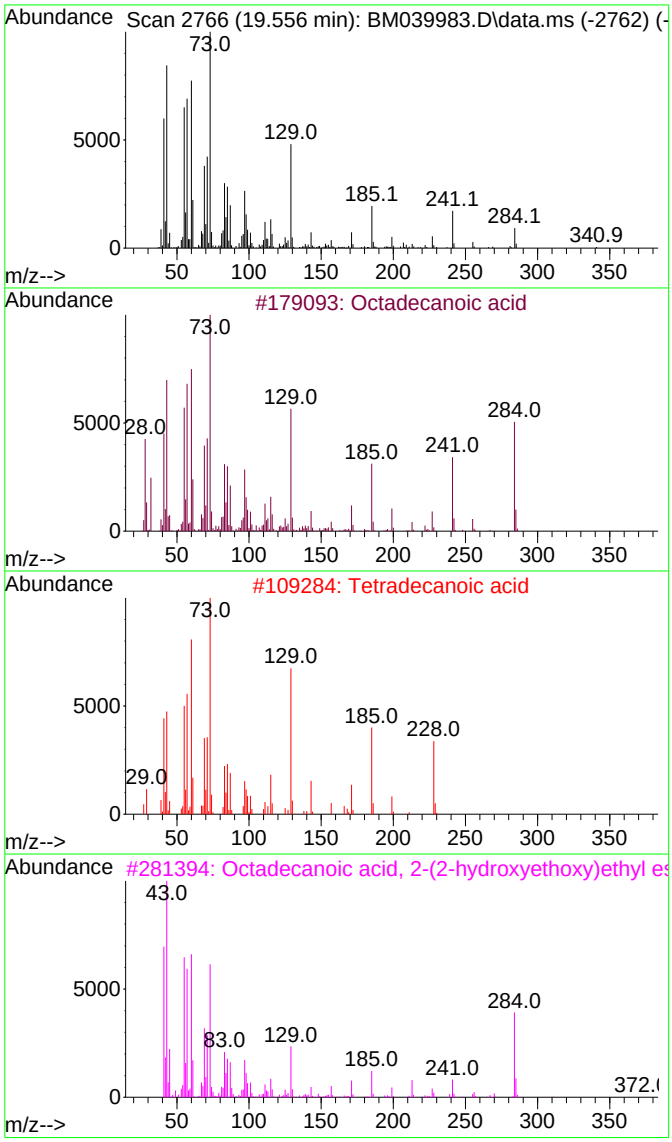
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

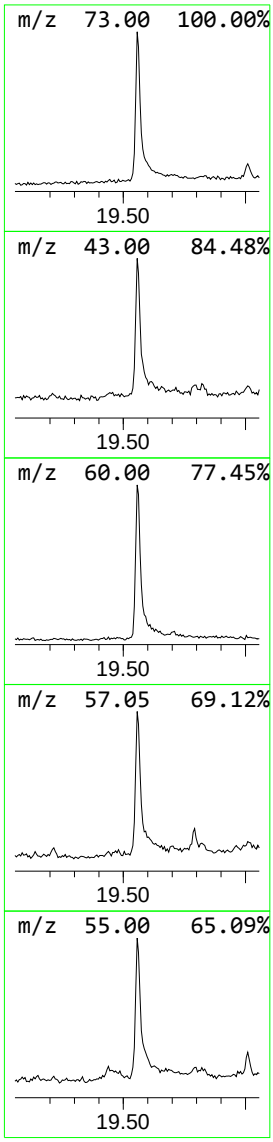
****

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.557	3.49 ng	683810	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

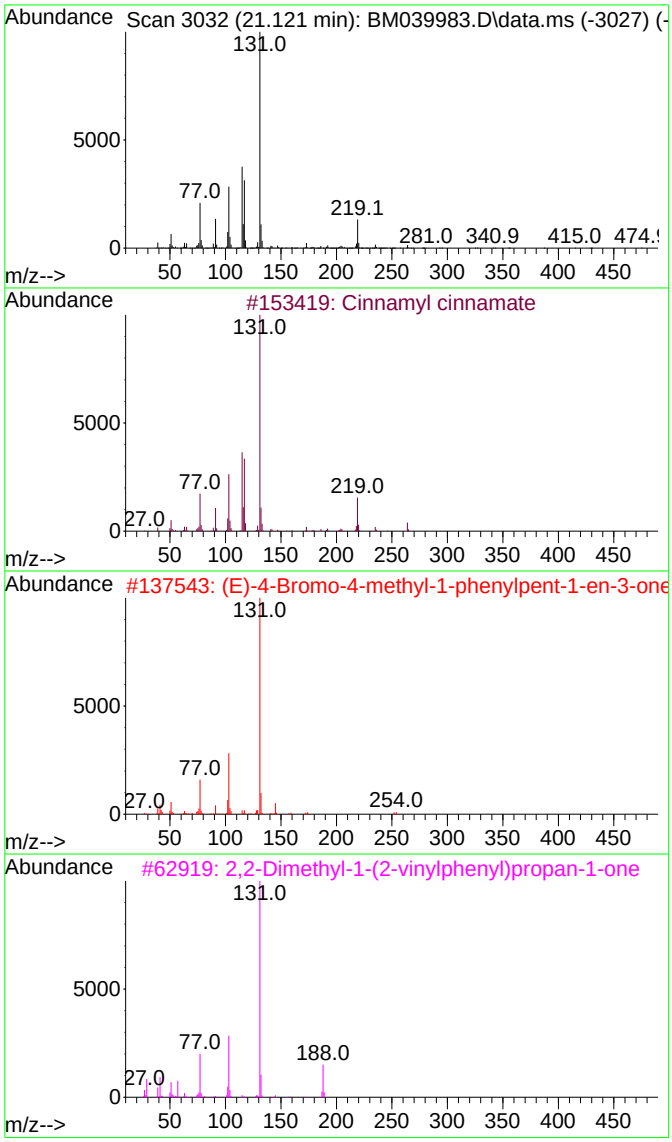
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

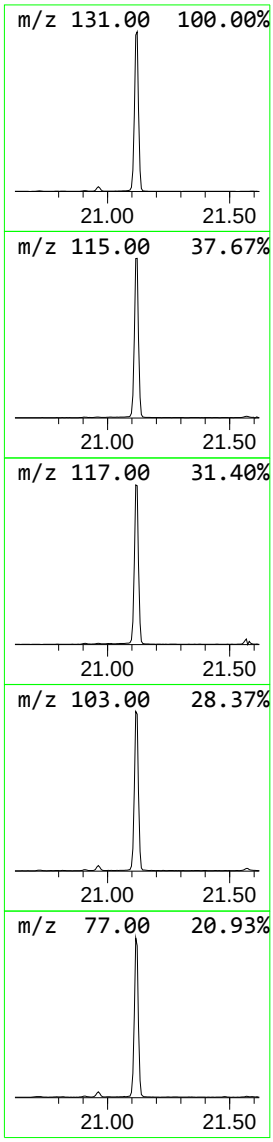
****

Peak Number 9 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	39.15 ng	7666030	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	53
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
4	N-(3-Chlorophenyl)-3-phenyl-2-pr...	257	C15H12ClNO	064741-15-7	50
5	Oxalic acid, monoamide monohydra...	323	C18H17N3O3	1000294-01-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

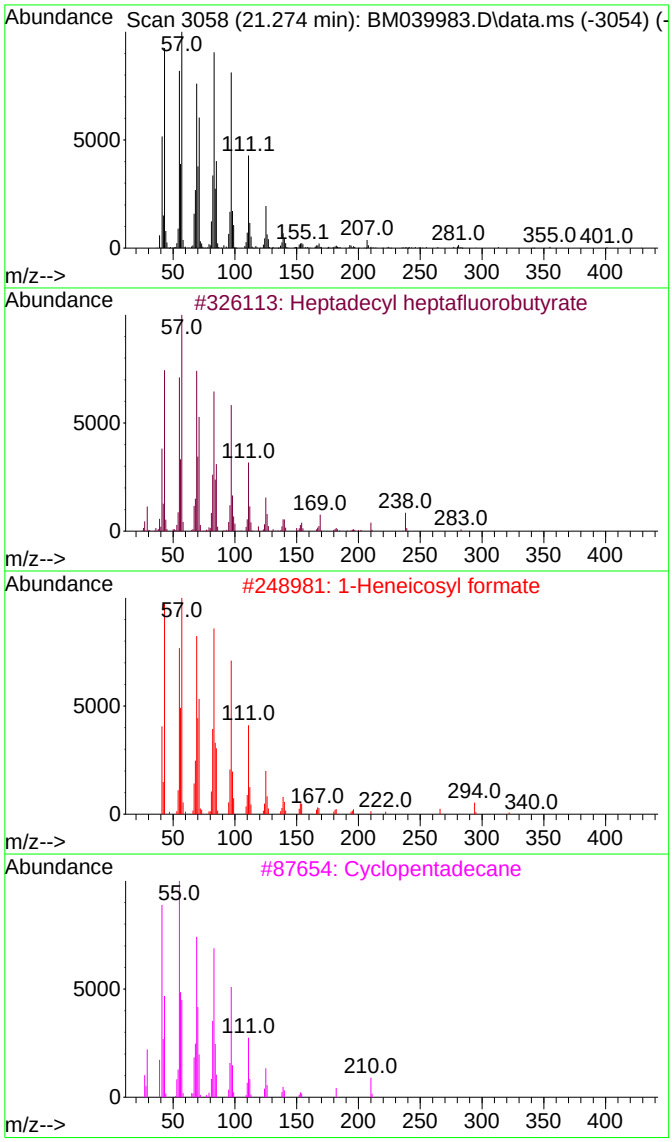
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

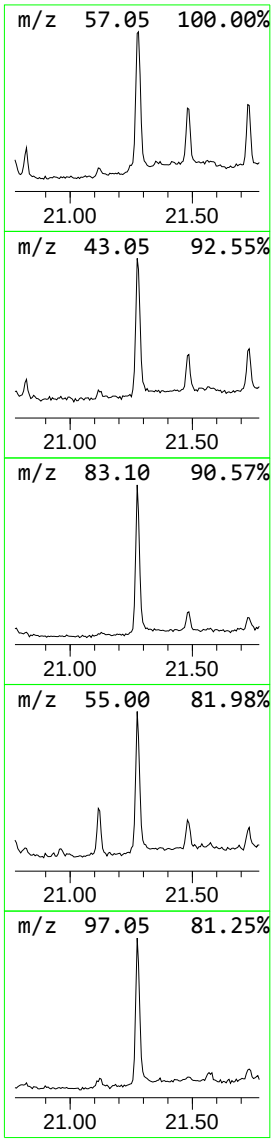
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.274	4.04 ng	791660	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039983.D
Acq On : 24 May 2023 14:33
Operator : CG/JU
Sample : 02868-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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
2-Pentanone, 4-...	5.093	5.3	ng	580909	1	8.016	2193150	20.0
(1S)-2,6,6-Trim...	6.693	5.0	ng	549341	1	8.016	2193150	20.0
Caryophyllene	13.980	8.4	ng	1320830	3	14.651	3128650	20.0
Humulene	14.369	2.7	ng	424264	3	14.651	3128650	20.0
1-Isopropyl-4,7...	14.904	2.9	ng	457561	3	14.651	3128650	20.0
Benzophenone	16.004	8.5	ng	1325280	3	14.651	3128650	20.0
n-Hexadecanoic ...	18.286	5.7	ng	926625	4	17.392	3238980	20.0
Octadecanoic acid	19.557	3.5	ng	683810	5	21.568	3916350	20.0
Cinnamyl cinnamate	21.121	39.1	ng	7666030	5	21.568	3916350	20.0
Heptadecyl hept...	21.274	4.0	ng	791660	5	21.568	3916350	20.0