LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040425\
Data File : BM049821.D
Acq On : 04 Apr 2025 13:25
Operator : RC/JU
Sample : Q1694-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-18

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-BM031325.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	3	5	14	rVB	182307	246276	1.16%	0.274%
2	4.904	320	326	337	rVB	1301155	1796891	8.45%	1.999%
3	5.369	398	405	414	rBV	5772538	7923824	37.26%	8.814%
4	5.981	503	509	518	rVB	232927	334934	1.57%	0.373%
5	6.957	666	675	686	rBV	5204143	8208116	38.60%	9.130%
6	7.786	808	816	822	rBV	973366	1472135	6.92%	1.638%
7	8.939	1004	1012	1022	rBV	3083914	4955286	23.30%	5.512%
8	10.580	1284	1291	1302	rBV	1139207	1855537	8.73%	2.064%
9	13.051	1703	1711	1727	rBV	8309425	12028567	56.56%	13.380%
10	14.427	1935	1945	1952	rBV	1708419	2481823	11.67%	2.761%
11	15.786	2167	2176	2183	rBV	1120697	1473118	6.93%	1.639%
12	15.915	2191	2198	2210	rBV	7538657	9973404	46.90%	11.094%
13	17.168	2405	2411	2417	rBV2	2119587	2912065	13.69%	3.239%
14	18.074	2558	2565	2574	rBV	1575698	2328365	10.95%	2.590%
15	18.339	2605	2610	2614	rBV	153582	238780	1.12%	0.266%
16	18.392	2615	2619	2632	rVV3	156589	357515	1.68%	0.398%
17	18.498	2633	2637	2650	rVB	237475	331658	1.56%	0.369%
18	19.350	2777	2782	2798	rBV	881727	1301236	6.12%	1.447%
19	19.797	2852	2858	2863	rBV	17982762	21266859	100.00%	23.656%
20	20.486	2972	2975	2983	rVB2	190681	220335	1.04%	0.245%
21	21.086	3073	3077	3089	rBV	445666	792151	3.72%	0.881%
22	21.403	3126	3131	3141	rVB	2498221	3462545	16.28%	3.852%
23	24.403	3634	3641	3657	rVB	1585909	3937639	18.52%	4.380%

Sum of corrected areas: 89899059

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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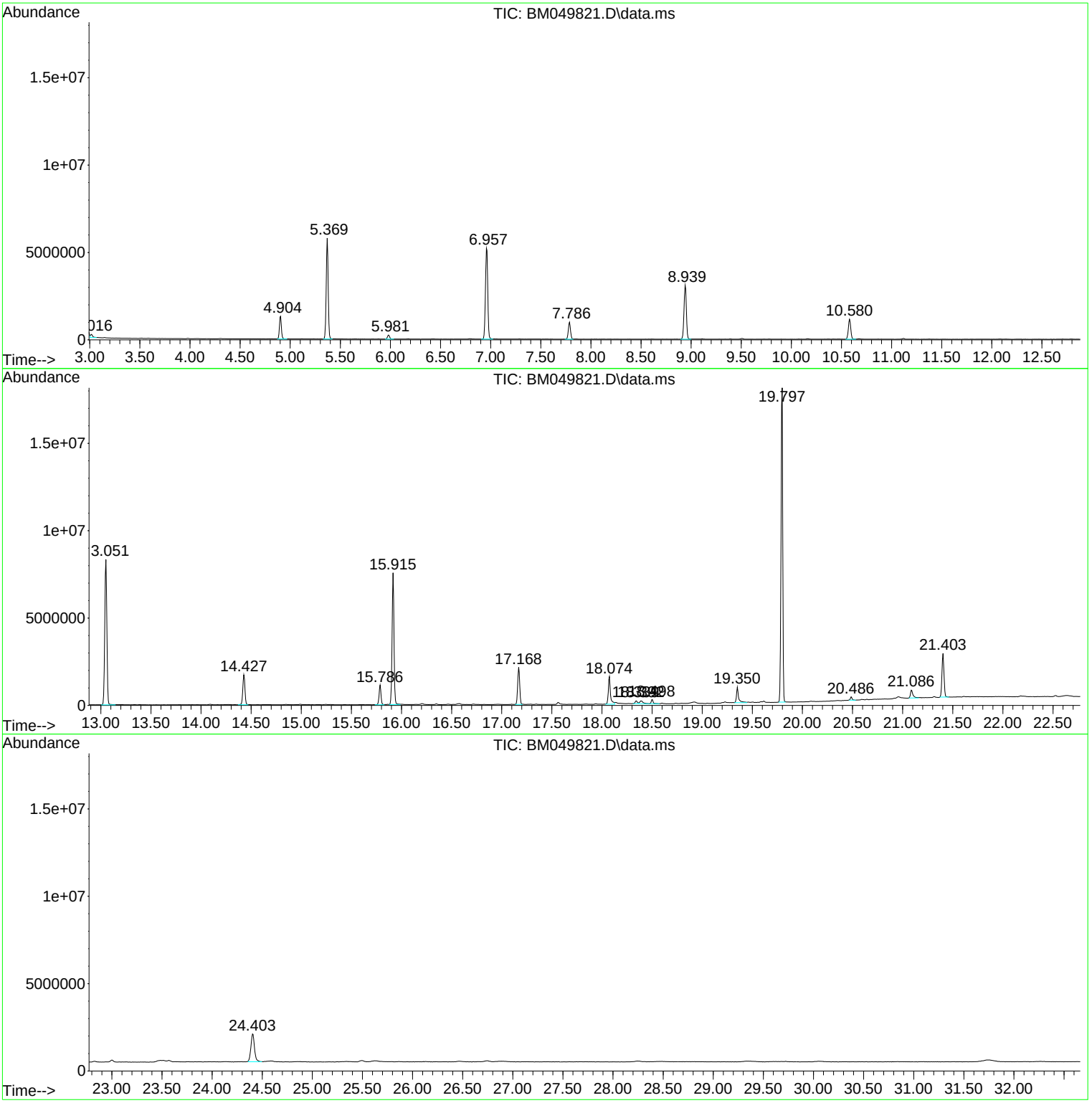
ClientSampleId :
TP-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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\BM040425\
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Acq On : 04 Apr 2025 13:25
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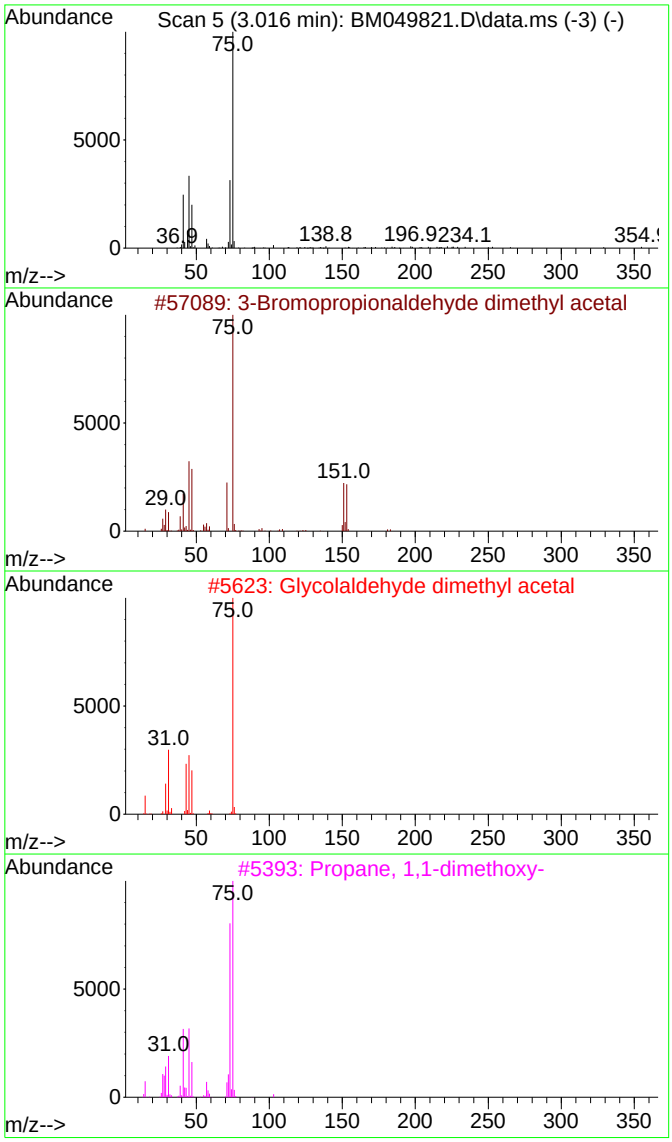
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

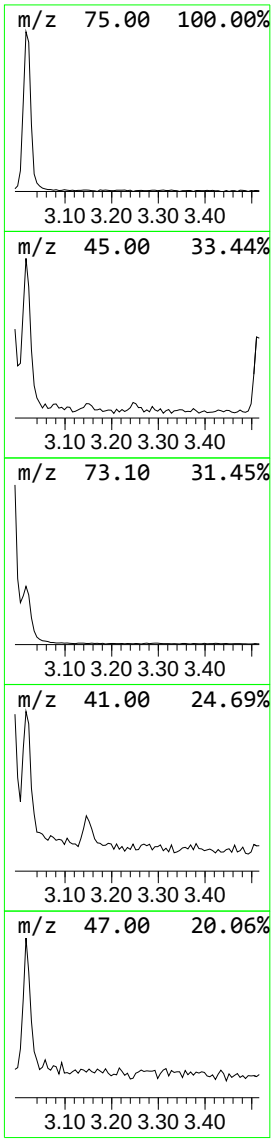
****

Peak Number 1 3-Bromopropionaldehyde dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	3.35 ng	246276	1,4-Dichlorobenzene-d4	7.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	64
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	50
3	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	39
4	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
5	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	38





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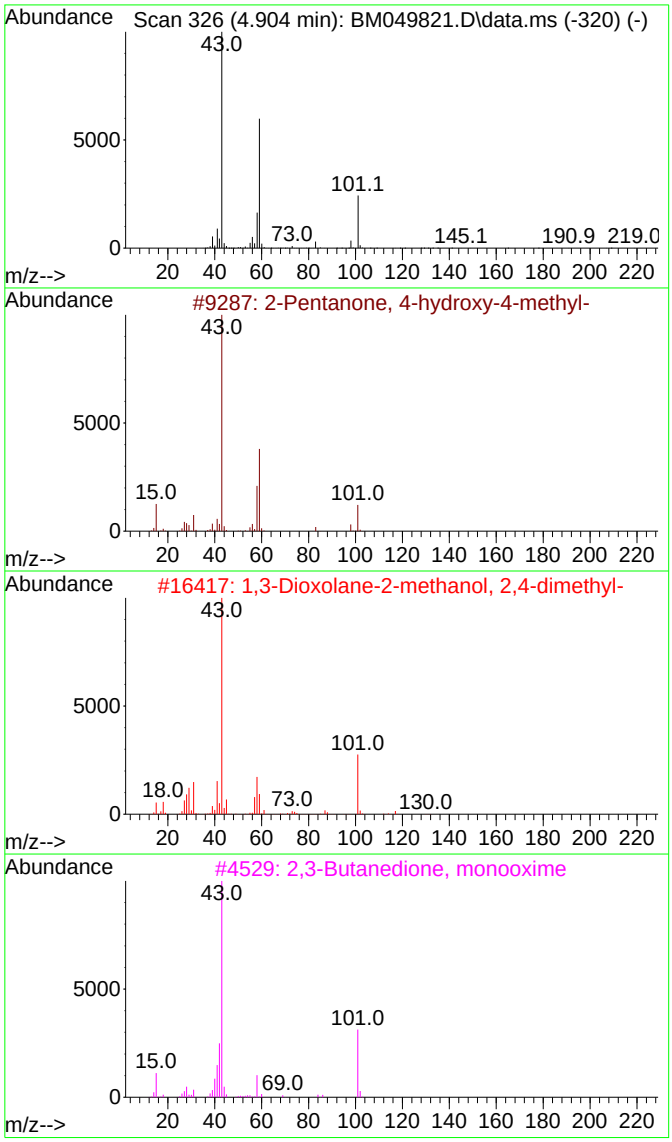
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

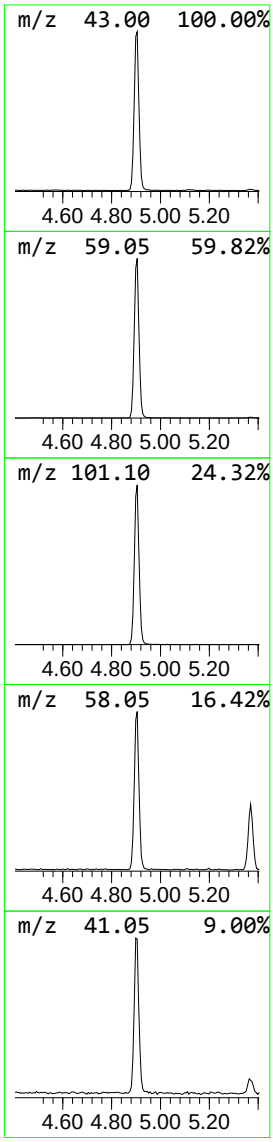
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	24.41 ng	1796890	1,4-Dichlorobenzene-d4	7.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Data File : BM049821.D
Acq On : 04 Apr 2025 13:25
Operator : RC/JU
Sample : Q1694-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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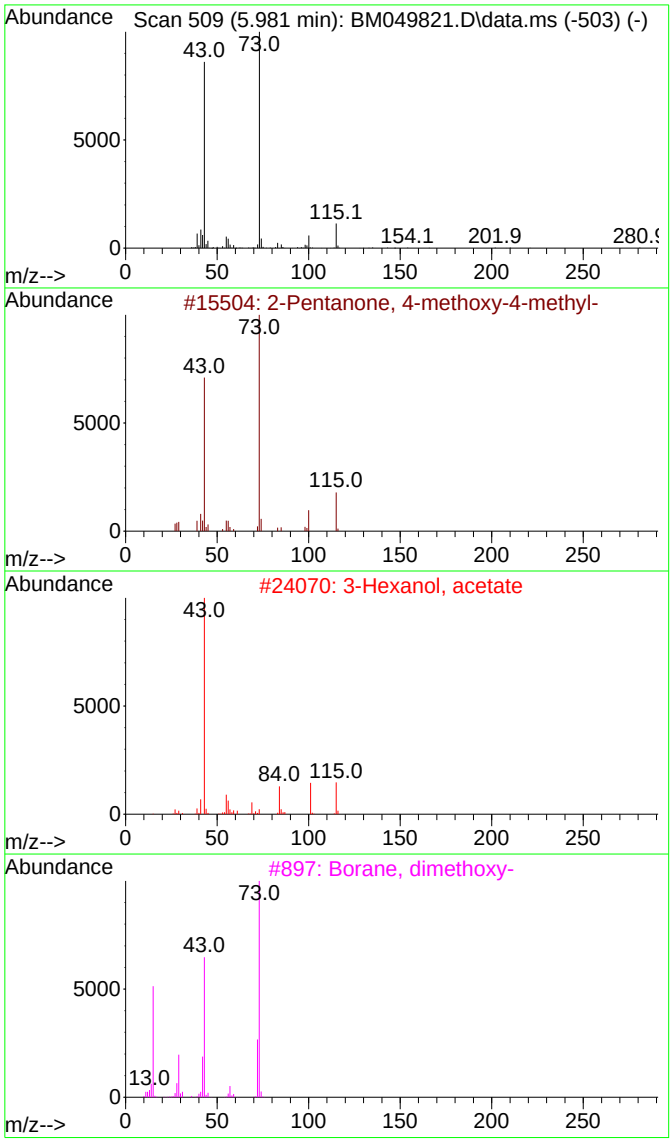
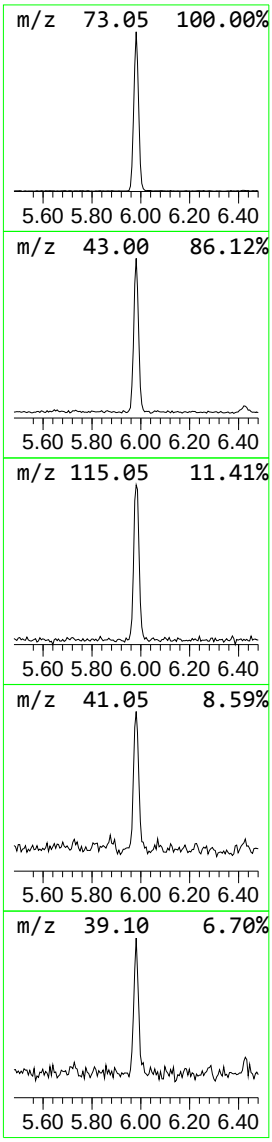
****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	4.55 ng	334934	1,4-Dichlorobenzene-d4	7.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	43
3	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	37
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
5	3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	23





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Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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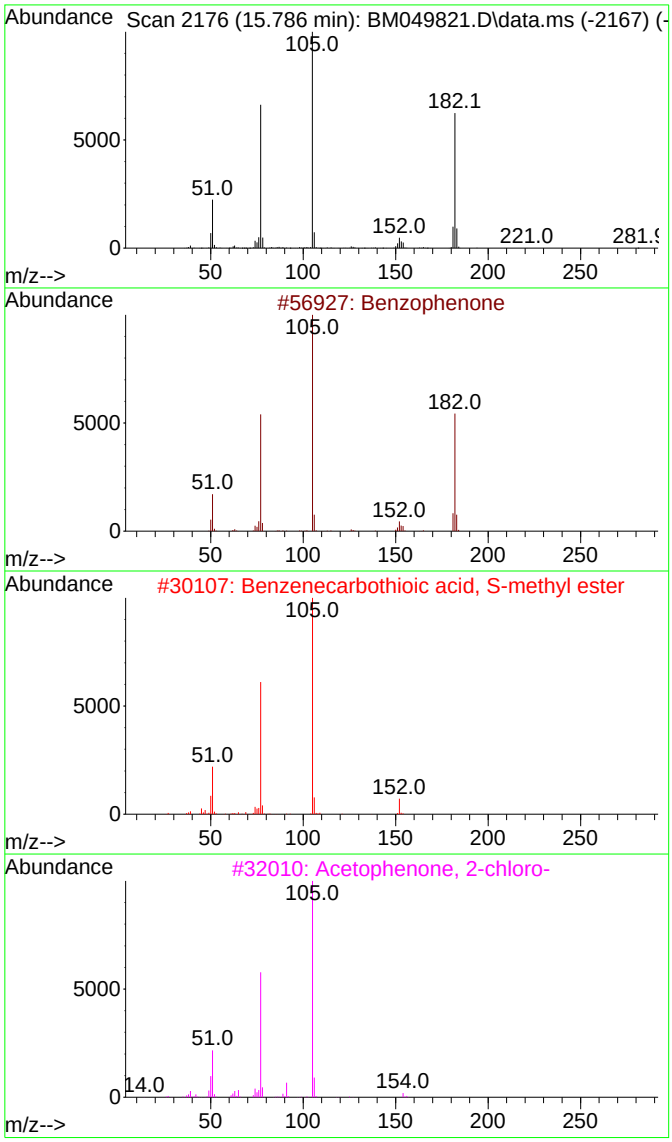
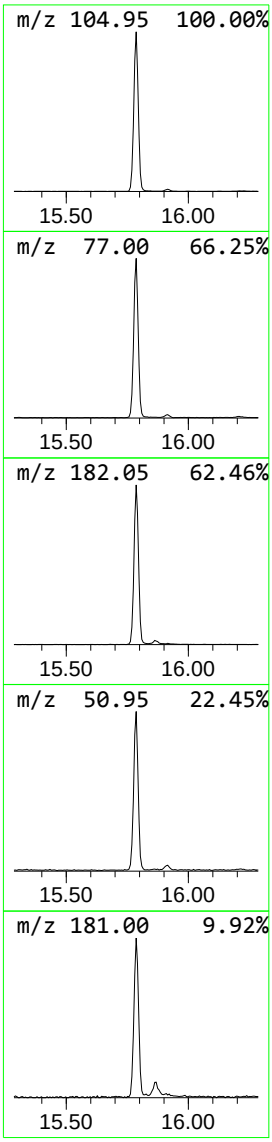
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	11.87 ng	1473120	Acenaphthene-d10	14.427

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	47
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
5	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	43





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

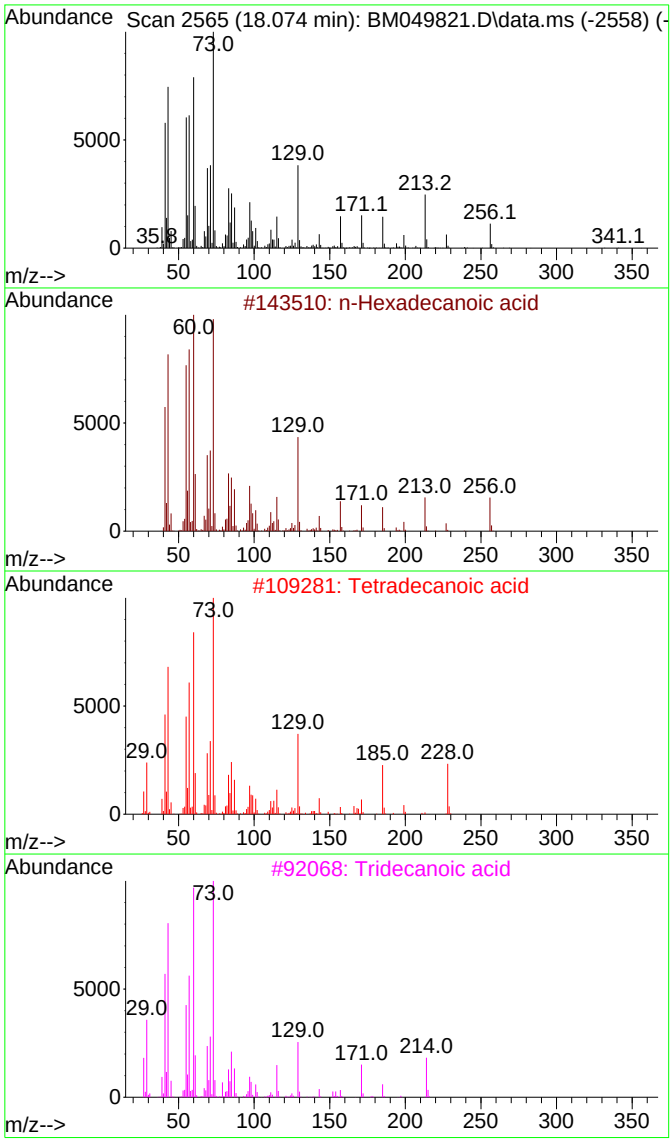
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

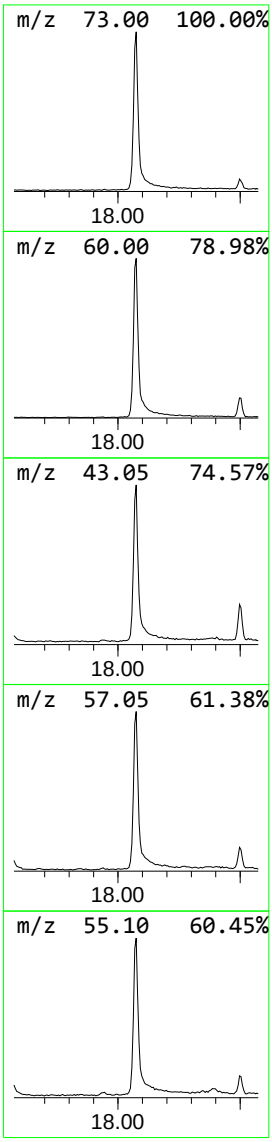
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	15.99 ng	2328370	Phenanthrene-d10	17.168

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	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	83





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

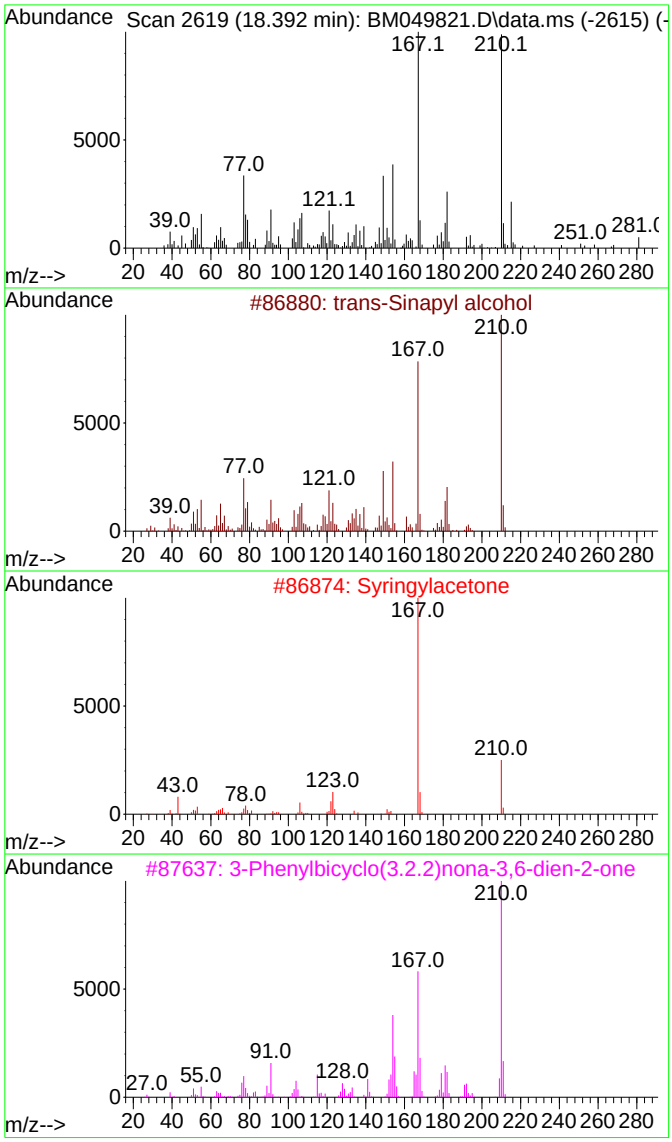
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

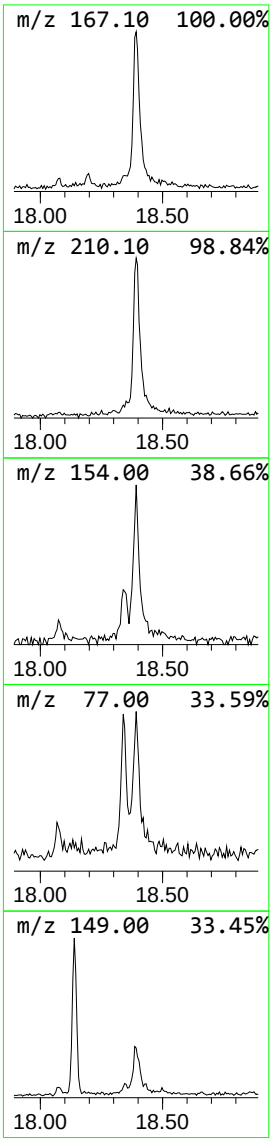
****

Peak Number 6 trans-Sinapyl alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.392	2.46 ng	357515	Phenanthrene-d10	17.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	97
2	Syringylacetone	210	C11H14O4	019037-58-2	49
3	3-Phenylbicyclo(3.2.2)nona-3,6-d...	210	C15H14O	073830-83-8	49
4	1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	43
5	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	43





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BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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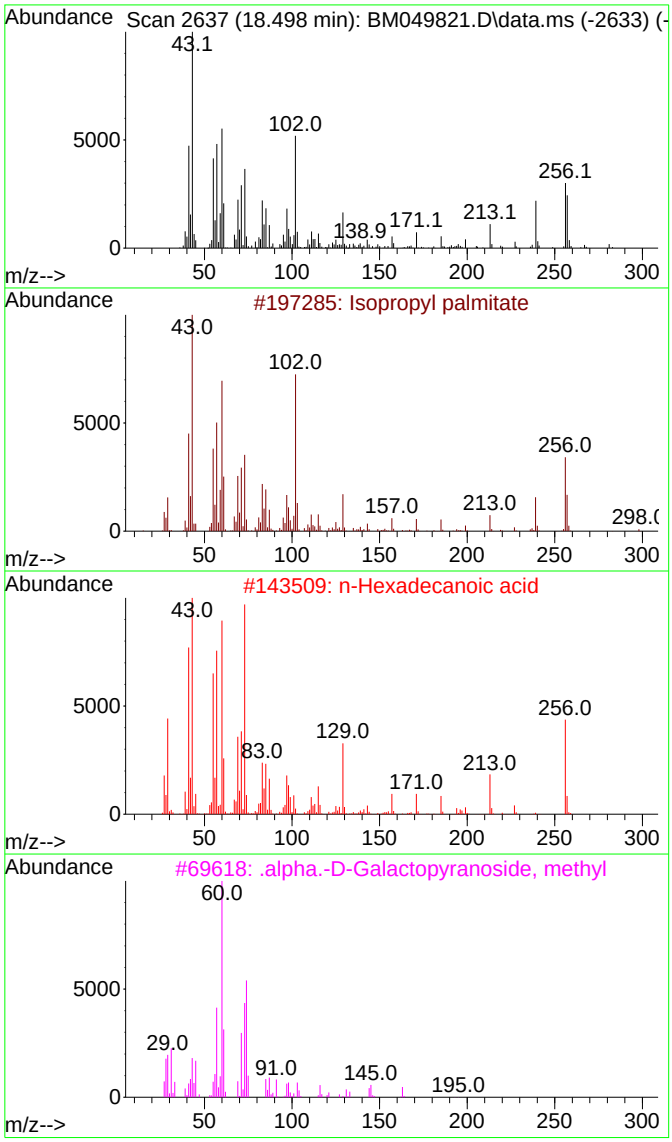
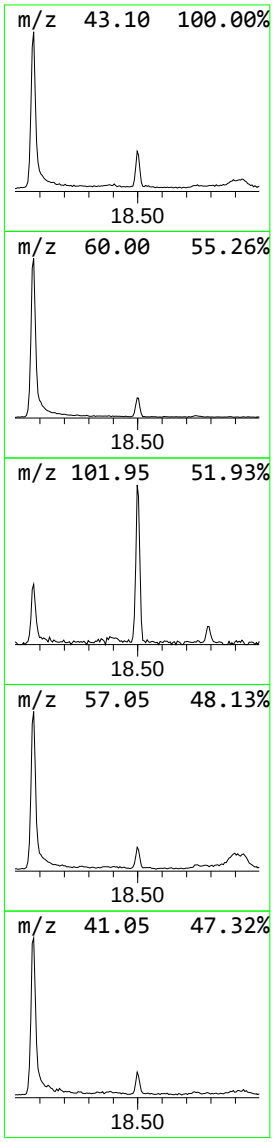
Peak Number 7 Isopropyl palmitate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.498	2.28 ng	331658	Phenanthrene-d10	17.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	72
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3	.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	27
4	Heptanoic acid, 2,2-dimethyl-6-o...	186	C10H18O3	000926-27-2	25
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	22





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TIC Library : C:\Database\NIST20.L
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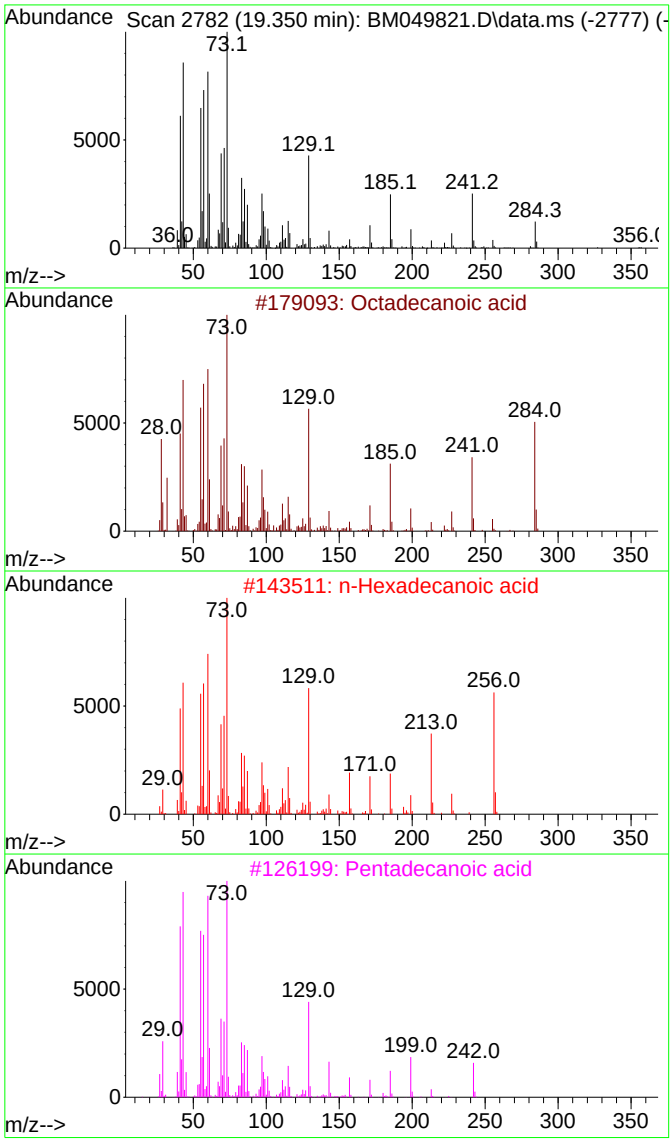
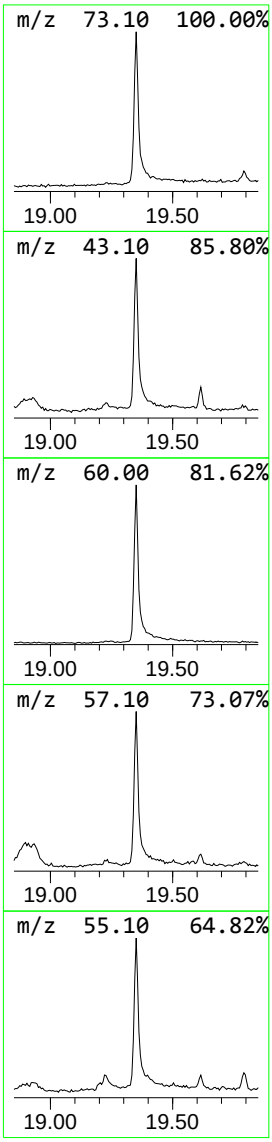
Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	7.52 ng	1301240	Chrysene-d12	21.403

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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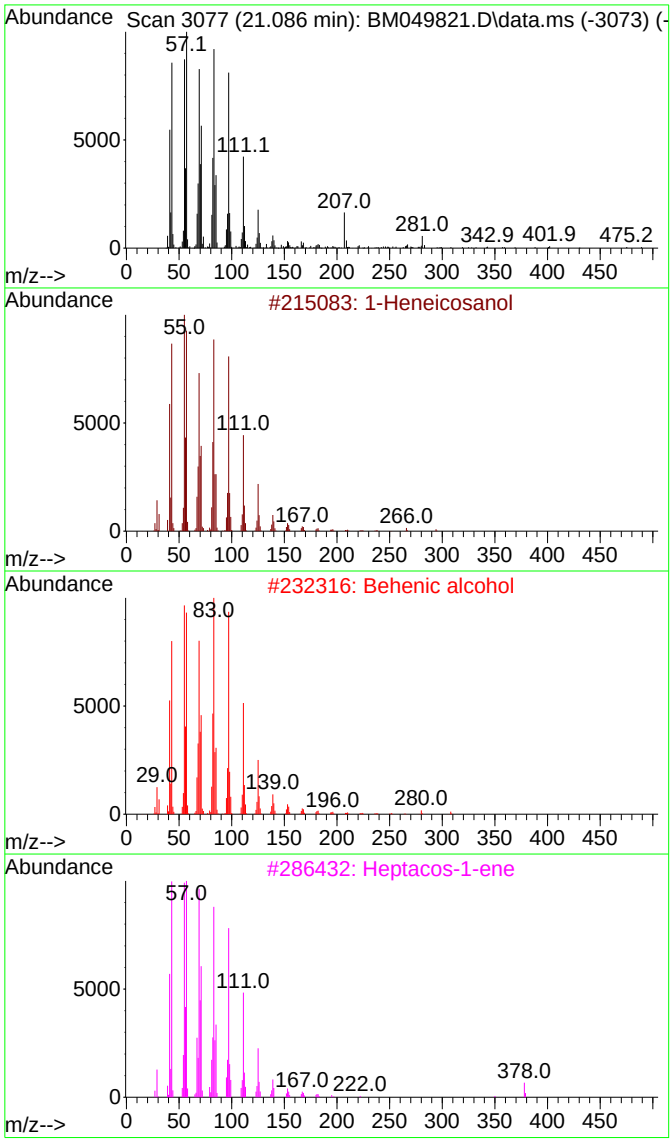
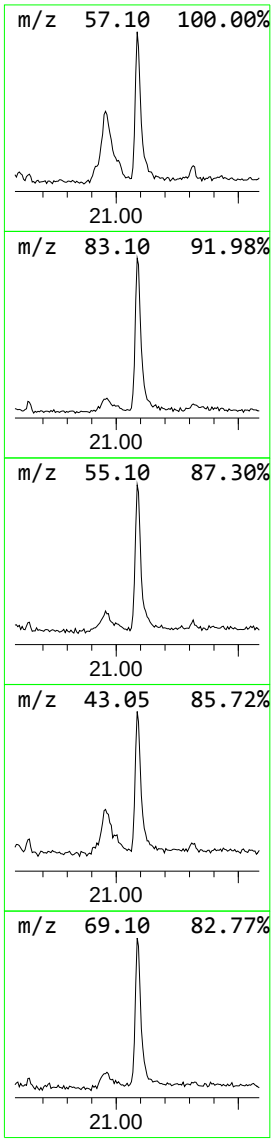
Peak Number 9 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	4.58 ng	792151	Chrysene-d12	21.403

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptacos-1-ene	378	C27H54	015306-27-1	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040425\
Data File : BM049821.D
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Operator : RC/JU
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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
3-Bromopropiona...	3.016	3.4	ng	246276	1	7.786	1472140	20.0
2-Pentanone, 4-...	4.904	24.4	ng	1796890	1	7.786	1472140	20.0
2-Pentanone, 4-...	5.981	4.5	ng	334934	1	7.786	1472140	20.0
Benzophenone	15.786	11.9	ng	1473120	3	14.427	2481820	20.0
n-Hexadecanoic ...	18.074	16.0	ng	2328370	4	17.168	2912070	20.0
trans-Sinapyl a...	18.392	2.5	ng	357515	4	17.168	2912070	20.0
Isopropyl palmi...	18.498	2.3	ng	331658	4	17.168	2912070	20.0
Octadecanoic acid	19.351	7.5	ng	1301240	5	21.403	3462550	20.0
1-Heneicosanol	21.086	4.6	ng	792151	5	21.403	3462550	20.0