LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041625\
Data File : BM049951.D
Acq On : 16 Apr 2025 14:07
Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

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-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.681	113	118	123	rBV	1022917	1283087	5.79%	0.830%
2	4.287	215	221	233	rBV	12167730	16712103	75.39%	10.816%
3	4.416	233	243	280	rBV	5597336	9653239	43.55%	6.247%
4	4.787	299	306	318	rVV6	100720	280658	1.27%	0.182%
5	5.357	396	403	419	rVB	7055202	10207367	46.05%	6.606%
6	6.916	662	668	671	rBV	6795604	10468656	47.23%	6.775%
7	6.951	671	674	698	rVB2	5189991	9000107	40.60%	5.825%
8	7.769	806	813	823	rBV	1567025	2493986	11.25%	1.614%
9	8.004	848	853	860	rVB	145290	240758	1.09%	0.156%
10	8.445	921	928	934	rBV	159721	261494	1.18%	0.169%
11	8.928	1002	1010	1022	rVB	4613098	7473546	33.71%	4.837%
12	9.263	1060	1067	1077	rBV	466560	1095047	4.94%	0.709%
13	9.363	1077	1084	1098	rVB	1394228	2467399	11.13%	1.597%
14	10.563	1280	1288	1301	rBV	1935844	3123360	14.09%	2.021%
15	11.857	1502	1508	1525	rVB	663021	1239693	5.59%	0.802%
16	12.416	1597	1603	1611	rVB	138331	245496	1.11%	0.159%
17	13.033	1699	1708	1718	rBV	12843915	18425434	83.12%	11.925%
18	13.851	1843	1847	1853	rBV	214364	328895	1.48%	0.213%
19	14.416	1936	1943	1953	rBV	1704032	2558180	11.54%	1.656%
20	14.986	2034	2040	2061	rBV3	201616	870226	3.93%	0.563%
21	15.174	2068	2072	2085	rBV5	122608	417512	1.88%	0.270%
22	15.904	2190	2196	2213	rBV	10315372	14960876	67.49%	9.682%
23	17.157	2403	2409	2418	rBV2	3283454	4766502	21.50%	3.085%
24	17.833	2519	2524	2536	rBV3	219562	441783	1.99%	0.286%
25	18.062	2557	2563	2591	rBV	3739083	6945614	31.33%	4.495%
26	19.339	2776	2780	2791	rBV	1171856	2081528	9.39%	1.347%
27	19.786	2850	2856	2862	rVB	18344503	22167101	100.00%	14.346%
28	20.480	2970	2974	2982	rVB2	490476	604908	2.73%	0.391%
29	21.397	3126	3130	3142	rVB2	1920623	3189197	14.39%	2.064%
30	22.509	3315	3319	3326	rVB2	325725	513170	2.32%	0.332%

Sum of corrected areas: 154516922

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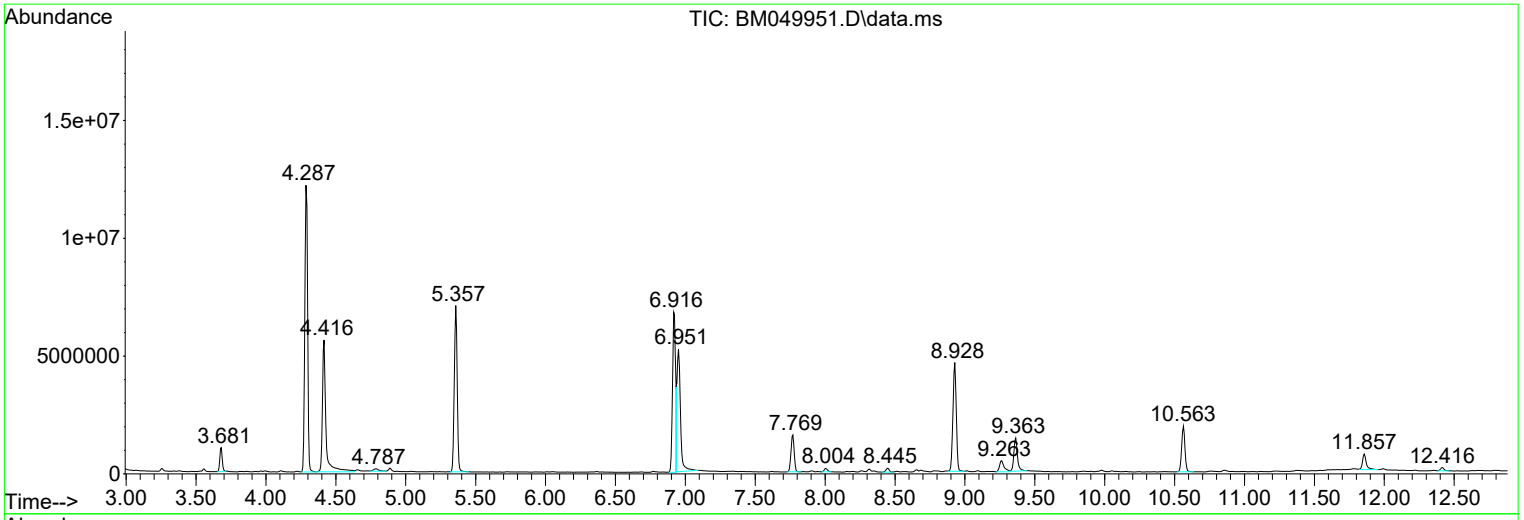
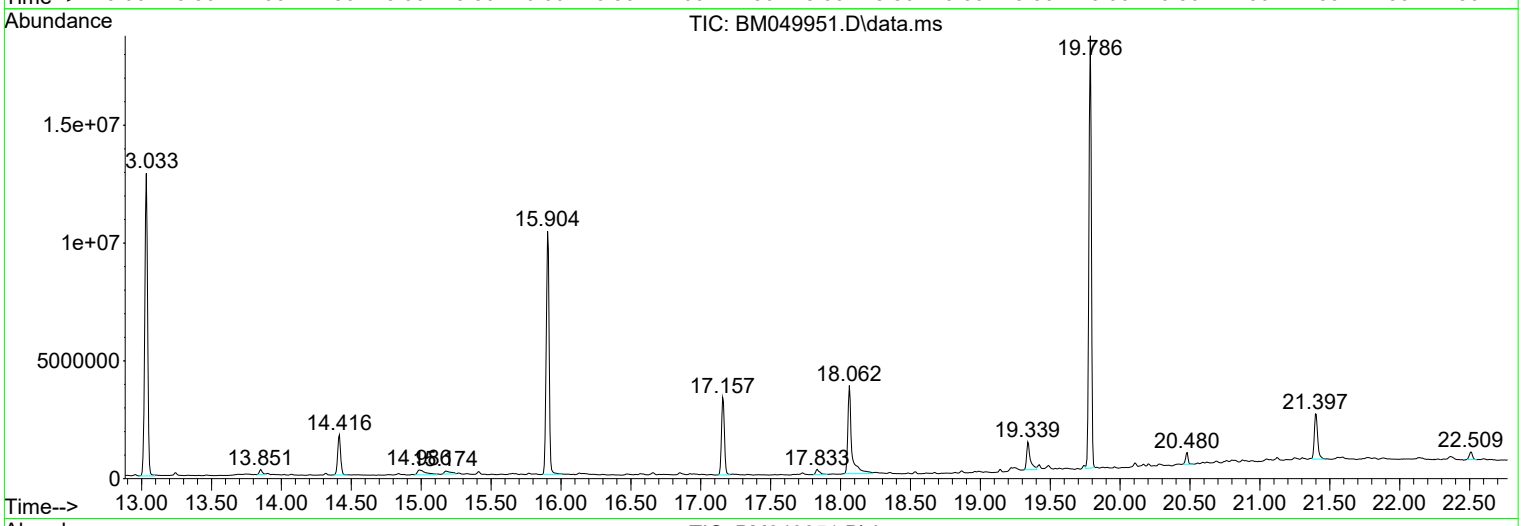
Misc :
ALS Vial : 9 Sample Multiplier: 1

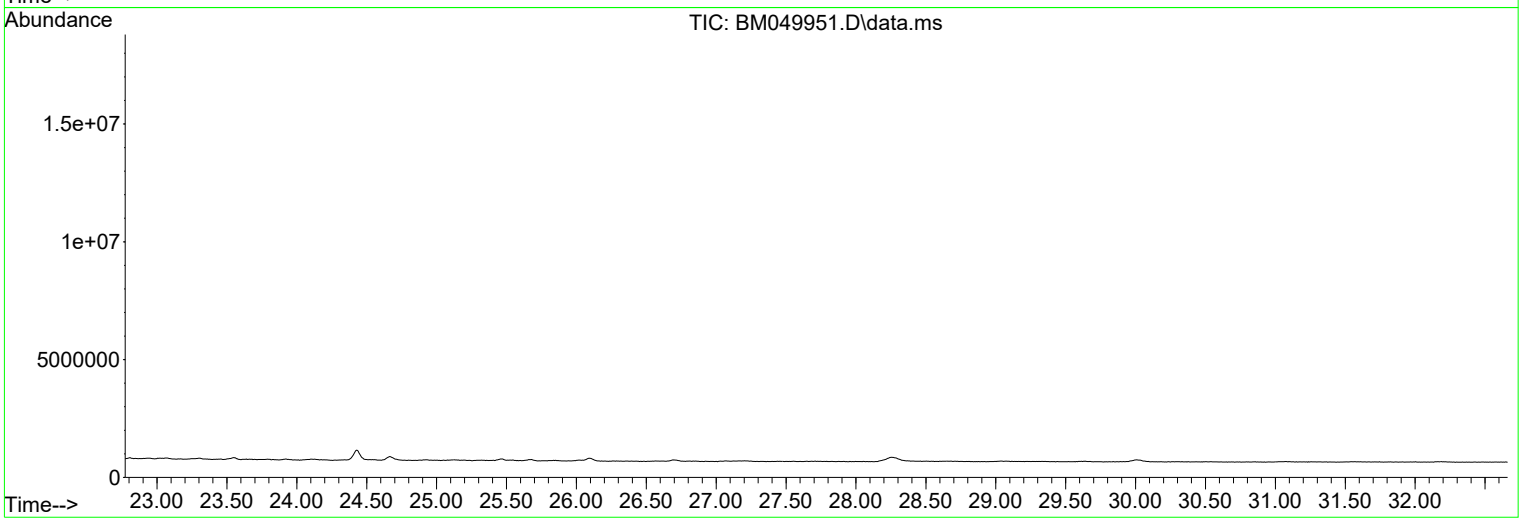
Instrument :
BNA_M
ClientSampleId :
279312

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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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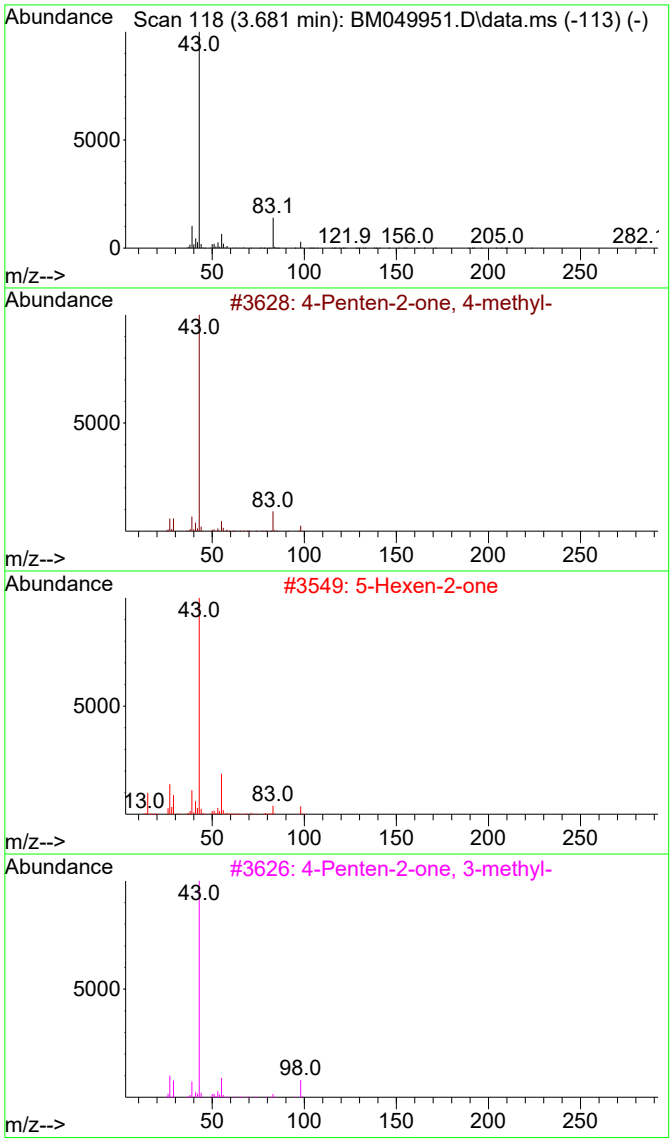
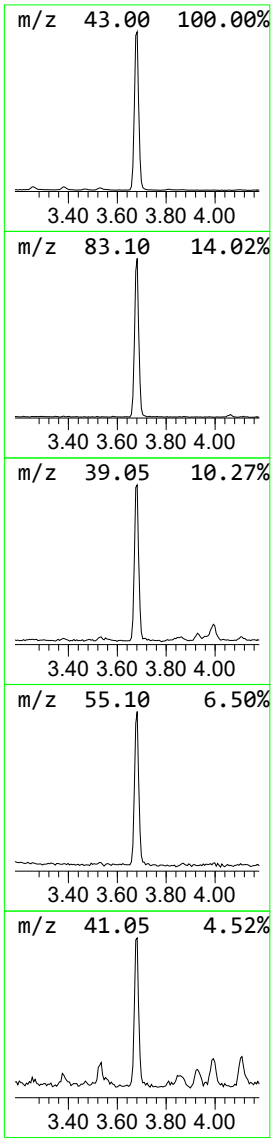
****
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	10.29 ng	1283090	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	53
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	53
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	35
5	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	25





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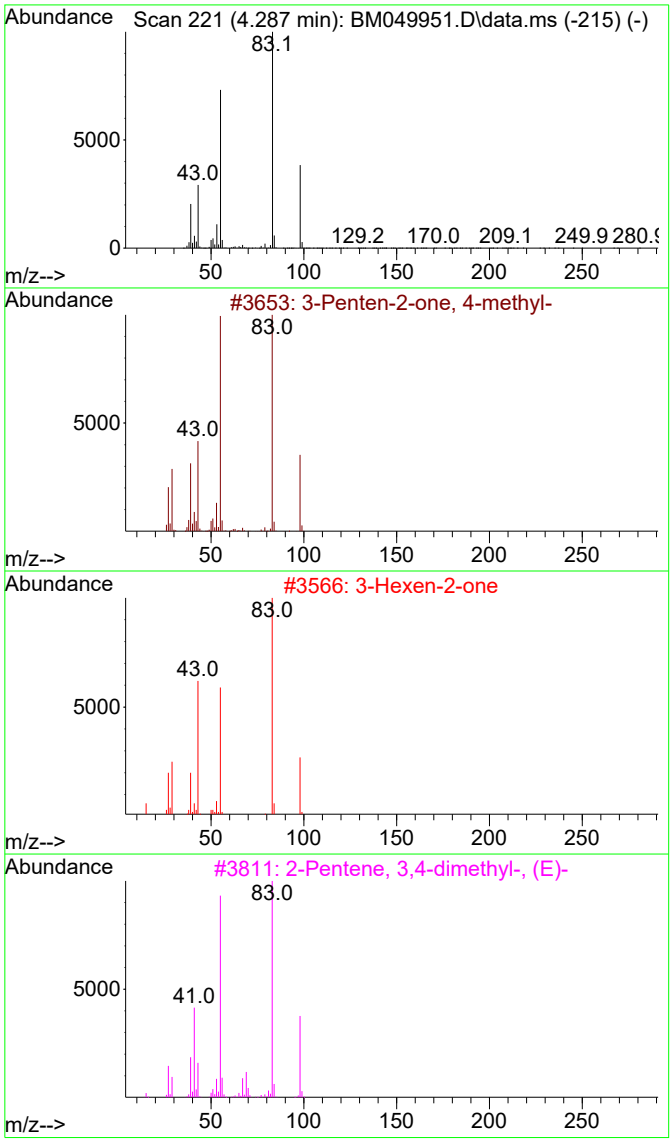
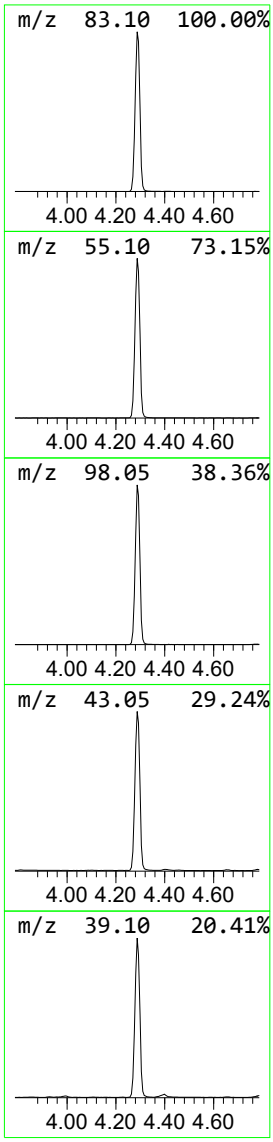
****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.287	134.02 ng	16712100	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78





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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
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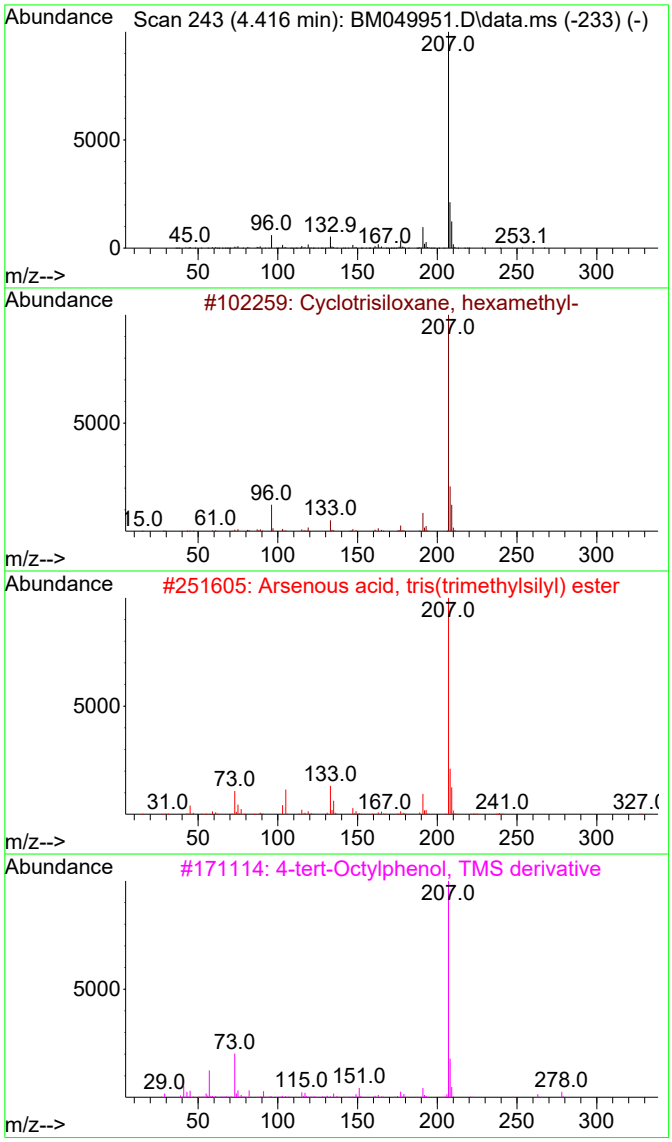
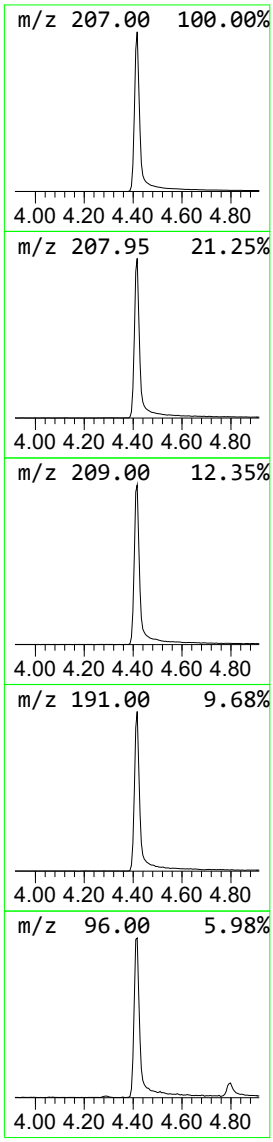
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	77.41 ng	9653240	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	64
3	4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	39
4	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39





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Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
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TIC Library : C:\Database\NIST20.L
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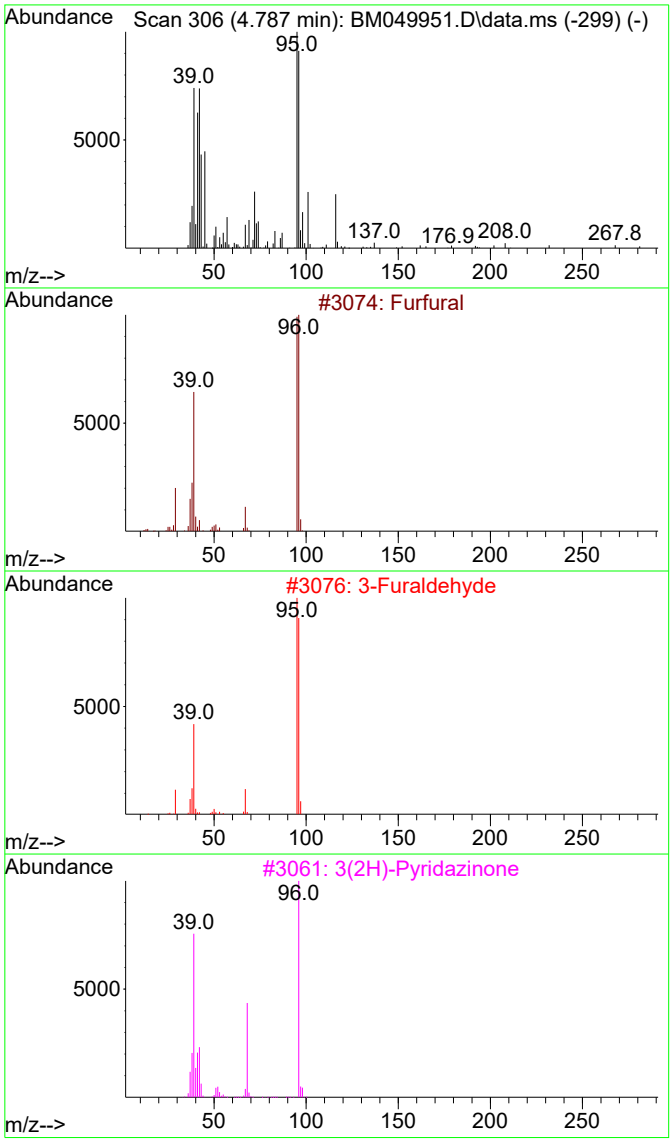
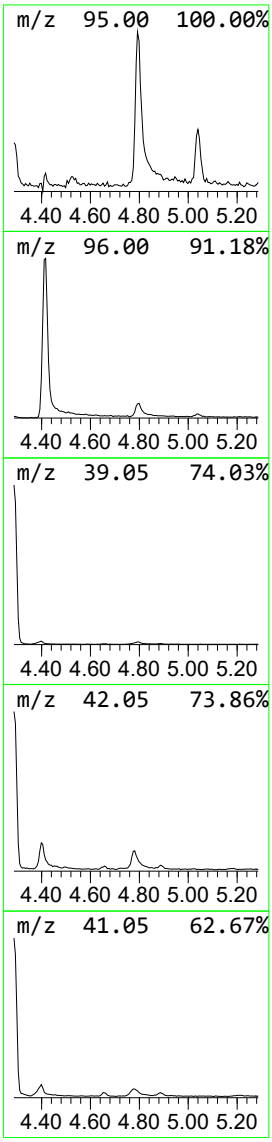
****
Peak Number 4 Furfural Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.787	2.25 ng	280658	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural	96	C5H4O2	000098-01-1	76
2	3-Furaldehyde	96	C5H4O2	000498-60-2	68
3	3(2H)-Pyridazinone	96	C4H4N2O	000504-30-3	58
4	2-Furancarboxylic acid, butyl ester	168	C9H12O3	000583-33-5	50
5	Propene	42	C3H6	000115-07-1	50





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
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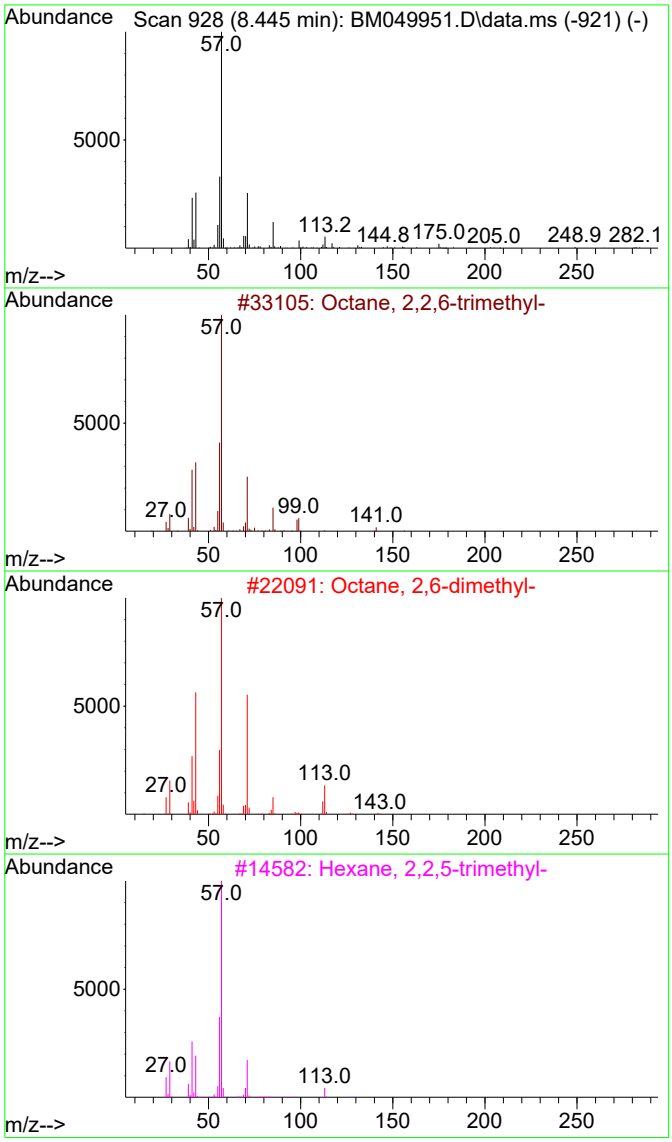
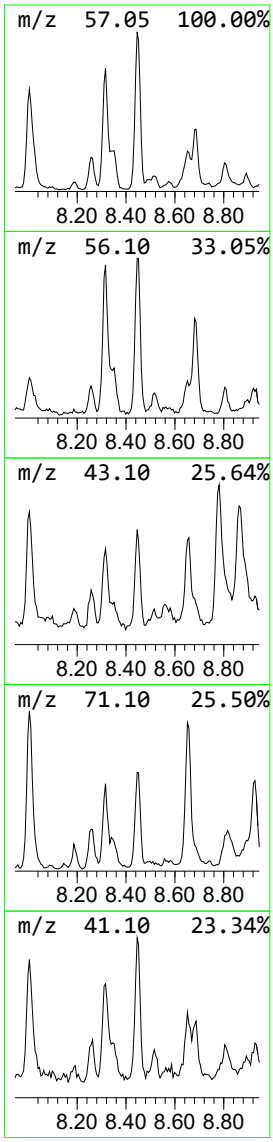
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octane, 2,2,6-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	2.10 ng	261494	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
3	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	53
4	Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	50
5	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	47





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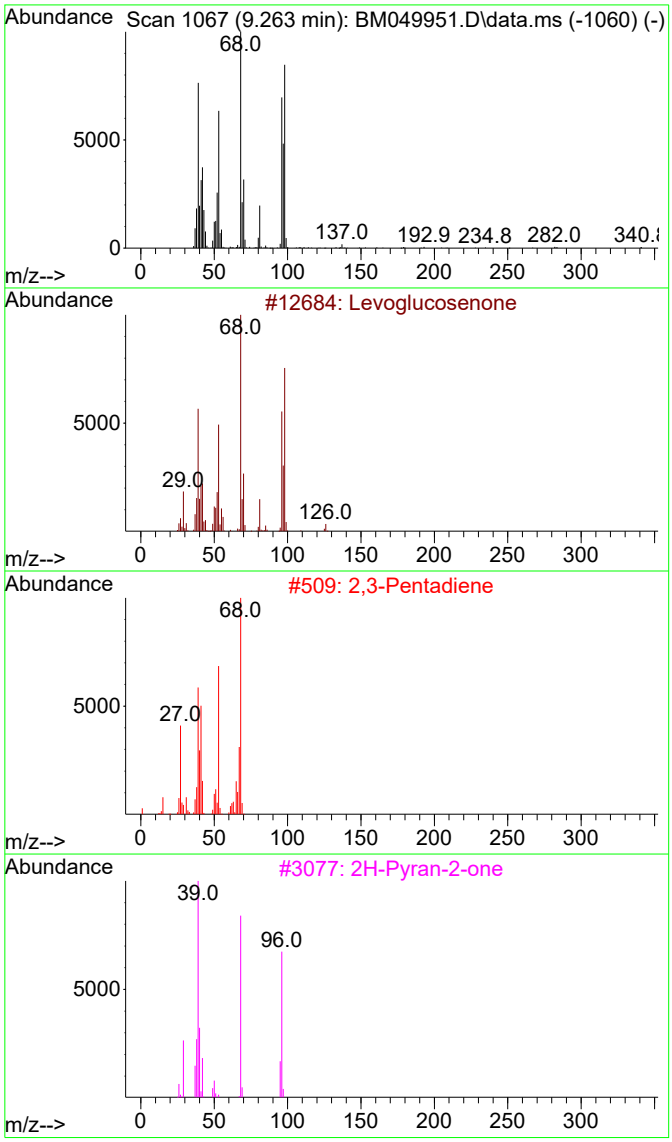
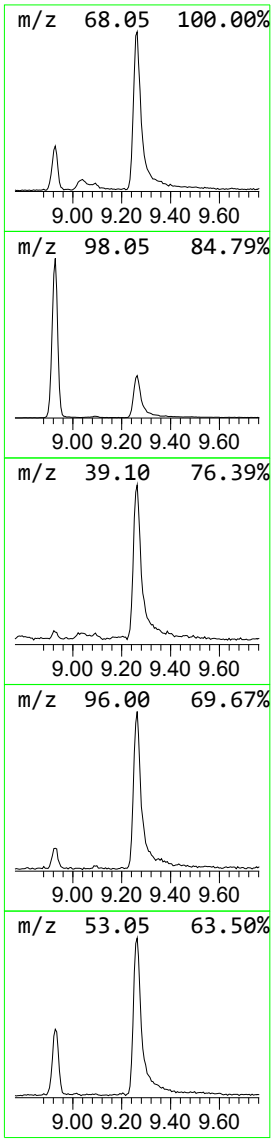
****

Peak Number 6 Levoglucosenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	7.01 ng	1095050	Naphthalene-d8	10.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levoglucosenone	126	C6H6O3	037112-31-5	87
2	2,3-Pentadiene	68	C5H8	000591-96-8	58
3	2H-Pyran-2-one	96	C5H4O2	000504-31-4	55
4	Bicyclo[3.1.0]hexan-3-one	96	C6H8O	001755-04-0	53
5	1,2-Pentadiene	68	C5H8	000591-95-7	50





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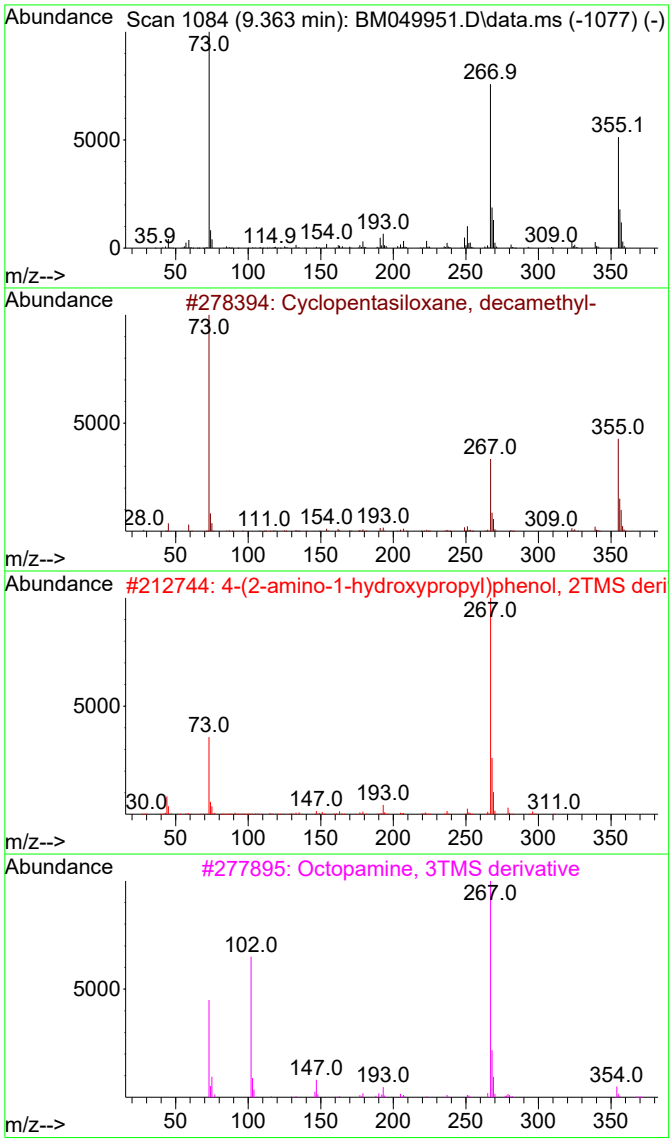
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

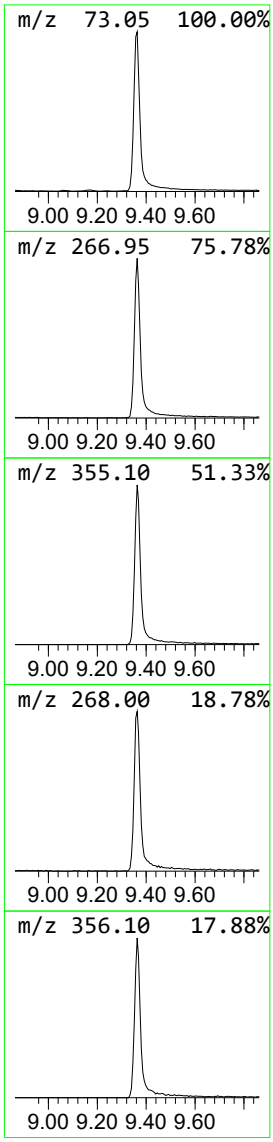
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	15.80 ng	2467400	Naphthalene-d8	10.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	91
2	4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	60
3	Octopamine, 3TMS derivative	369	C17H35NO2Si3	068595-60-8	50
4	3-Hydroxymandelic acid, 3TMS der...	384	C17H32O4Si3	068595-69-7	47
5	p-Trimethylsilyloxyphenyl-bis(tr...	370	C17H34O3Si3	1000079-08-1	47





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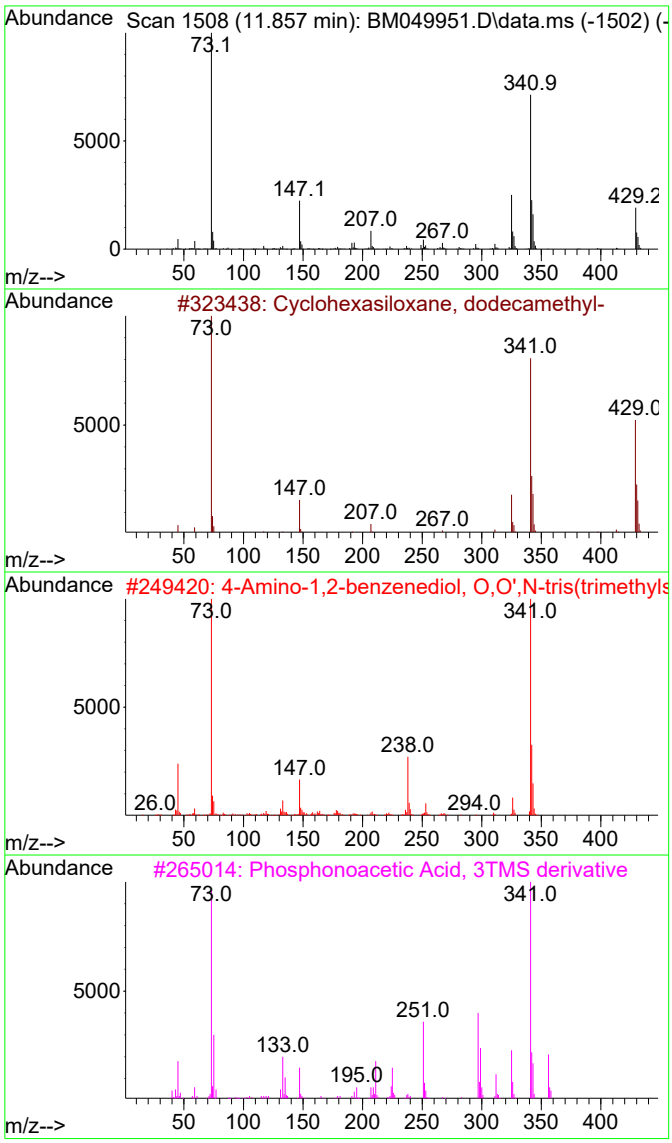
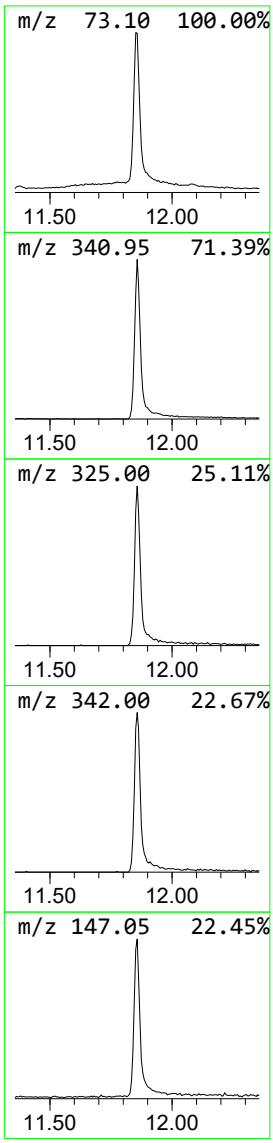
****
Peak Number 8 Cyclohexasiloxane, dodecame... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.94 ng	1239690	Naphthalene-d8	10.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	90
2	4-Amino-1,2-benzenediol, O,O',N-...	341	C15H31NO2Si3	1000493-87-4	53
3	Phosphonoacetic Acid, 3TMS deriv...	356	C11H29O5PSi3	053044-27-2	50
4	4,6'-Dimethoxy-2'-(tert.-butyldi...	398	C23H30O4Si	1010454-23-8	38
5	2,5'-Dimethoxy-2'-(trimethylsily...	356	C20H24O4Si	1000454-26-6	38





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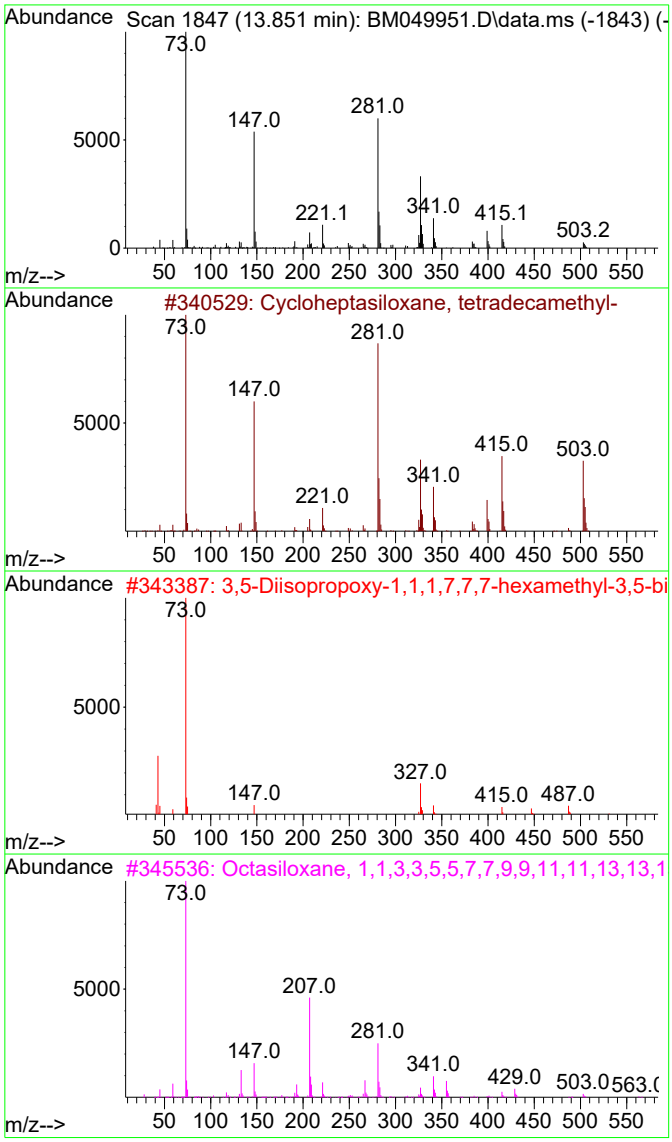
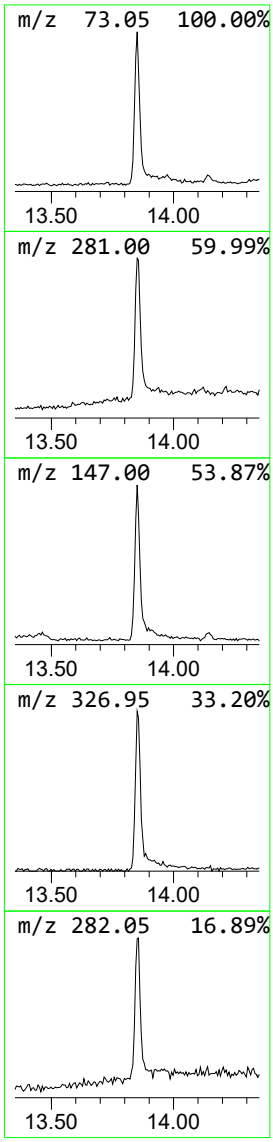
****
Peak Number 9 Cycloheptasiloxane, tetrade... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.57 ng	328895	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	93
2	3,5-Diisopropoxy-1,1,1,7,7,7-hex...	546	C18H50O7Si6	071579-67-4	27
3	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	25
4	2-(14-Carboxytetradecyl)-2-ethyl...	384	C22H42NO4	053034-38-1	22
5	Benzamide, 4-propyl-N-octadecyl-	415	C28H49NO	1000439-17-9	22





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Data File : BM049951.D
Acq On : 16 Apr 2025 14:07
Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

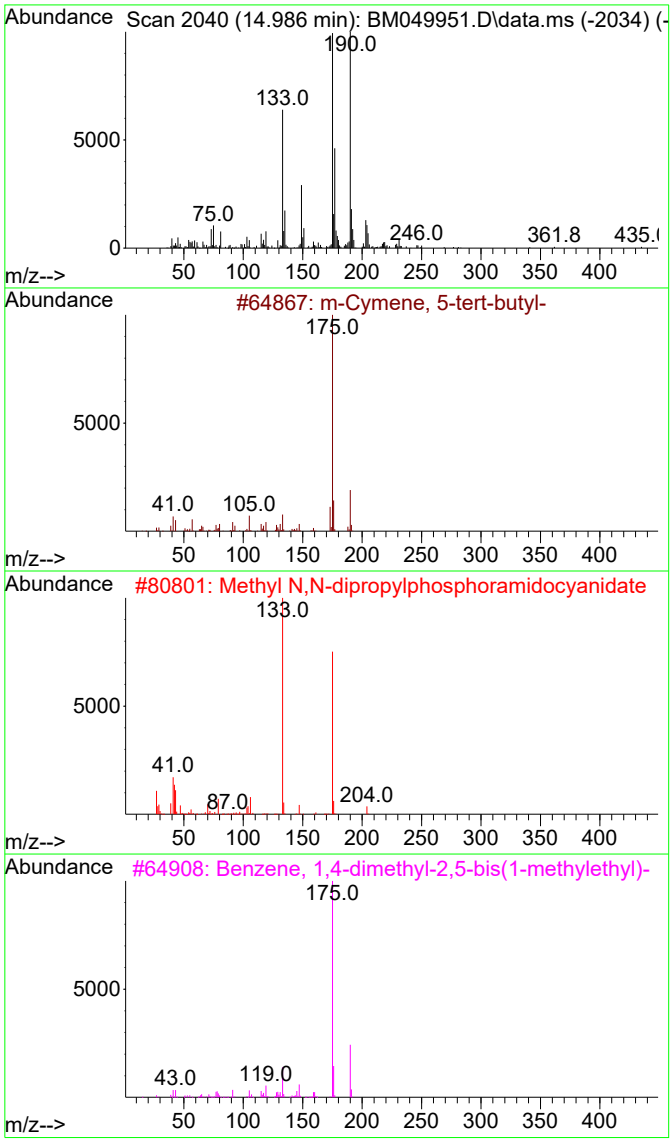
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

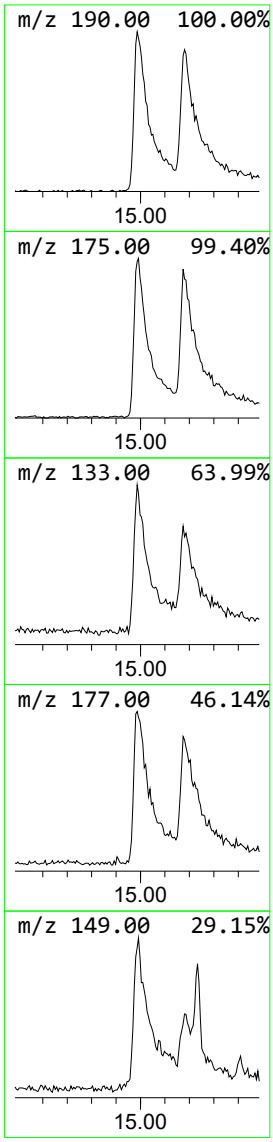
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 m-Cymene, 5-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	6.80 ng	870226	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Cymene, 5-tert-butyl-	190	C14H22	029577-19-3	50
2	Methyl N,N-dipropylphosphoramido...	204	C8H17N2O2P	1000298-42-0	35
3	Benzene, 1,4-dimethyl-2,5-bis(1-...	190	C14H22	010375-96-9	35
4	5-Fluoro-4-chloro-2-dimethylamin...	175	C6H7ClFN3	1000070-49-0	35
5	Pyrazol-5(4H)-one, 3-(4-methoxyp...	190	C10H10N2O2	001578-89-8	35





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Acq On : 16 Apr 2025 14:07
Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

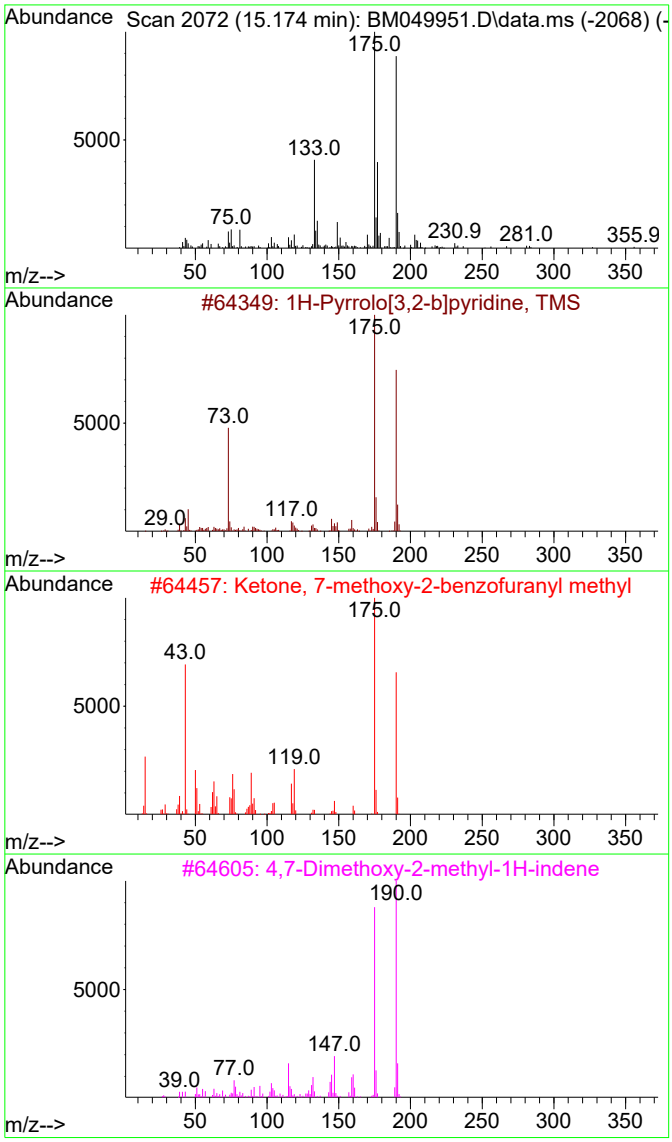
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

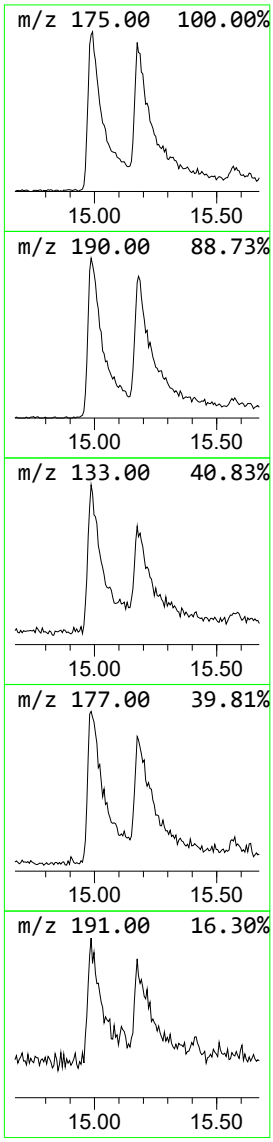
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1H-Pyrrolo[3,2-b]pyridine, TMS Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.26 ng	417512	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrolo[3,2-b]pyridine, TMS	190	C10H14N2Si	1000504-23-2	50
2	Ketone, 7-methoxy-2-benzofuranyl...	190	C11H10O3	043071-52-9	38
3	4,7-Dimethoxy-2-methyl-1H-indene	190	C12H14O2	1000188-03-2	38
4	Dicyclanil	190	C8H10N6	112636-83-6	38
5	[2,2'-Bifuran]-5,5'-dicarboxalde...	190	C10H6O4	005905-01-1	35





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Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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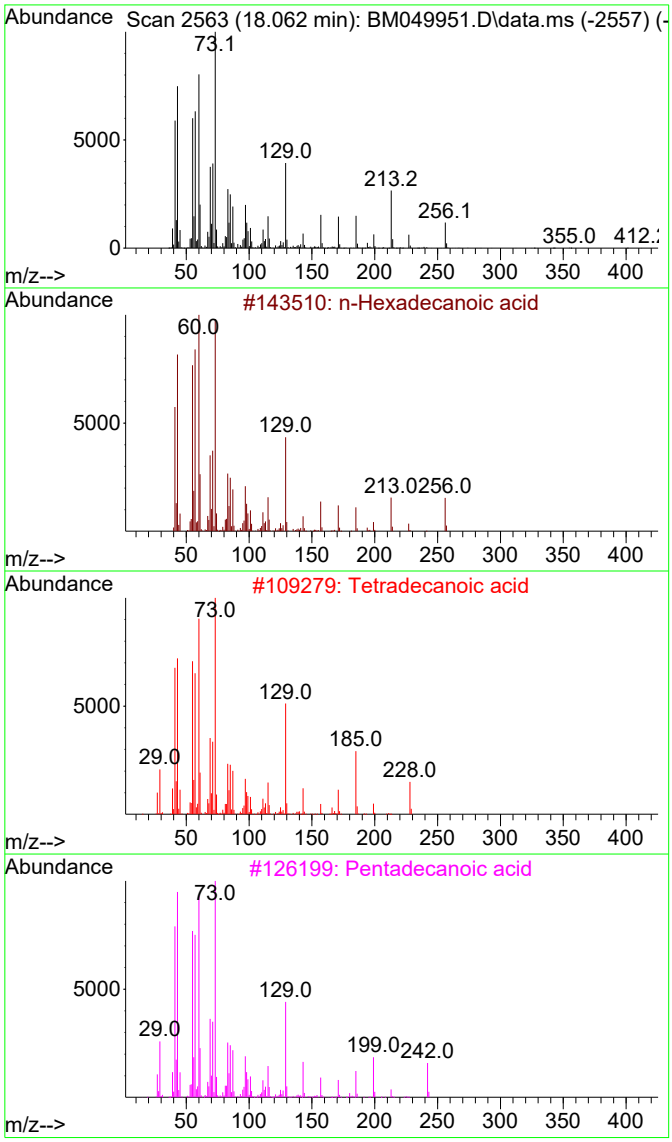
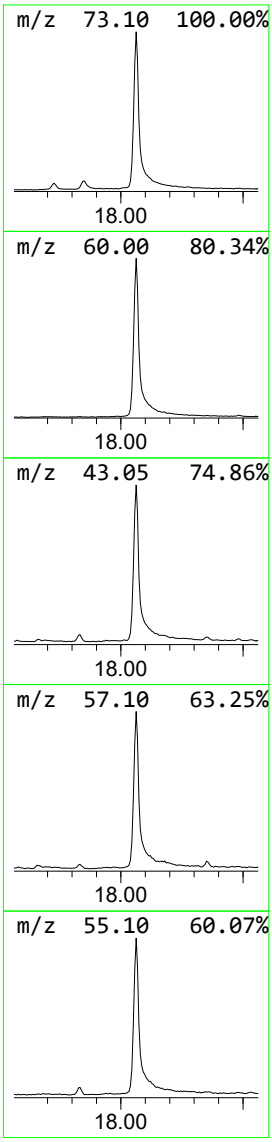
****

Peak Number 12 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	29.14 ng	6945610	Phenanthrene-d10	17.157

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

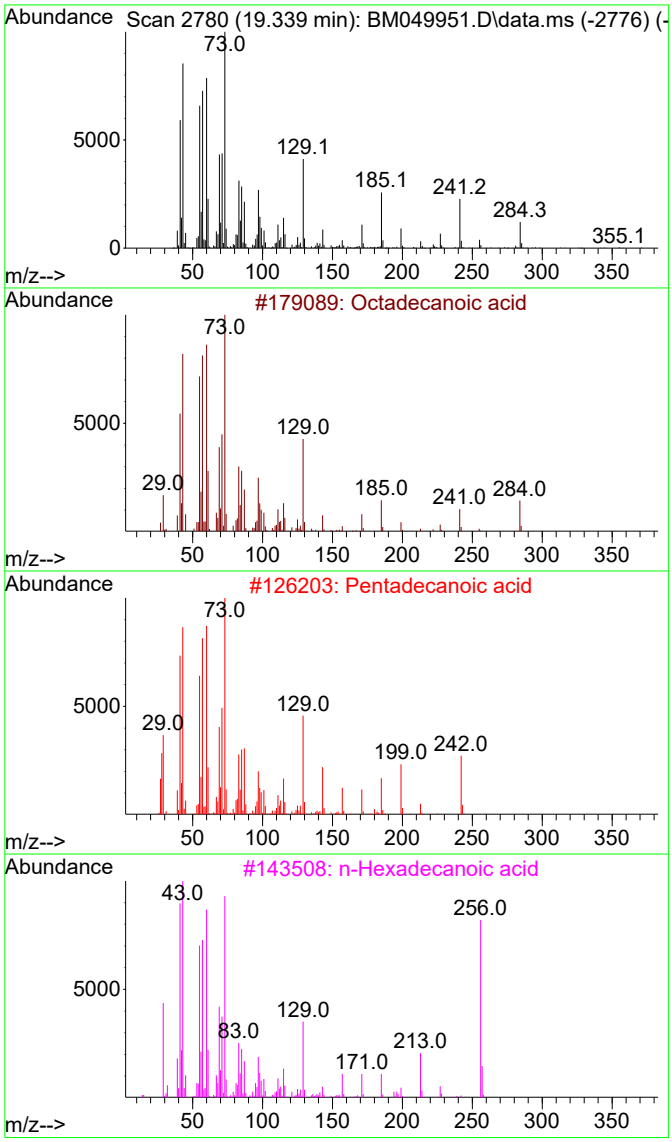
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

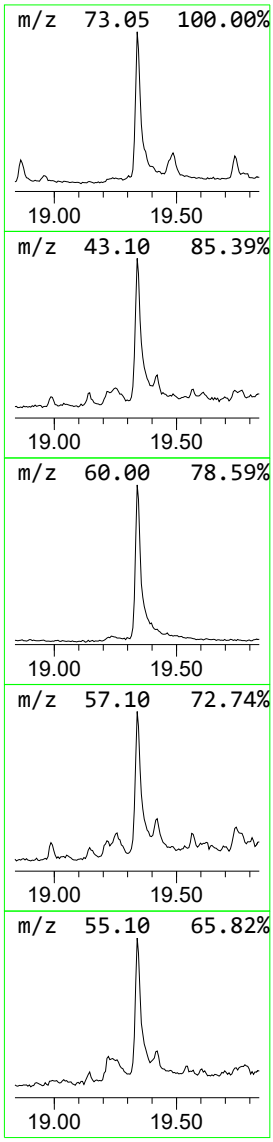
****

Peak Number 13 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	13.05 ng	2081530	Chrysene-d12	21.397

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

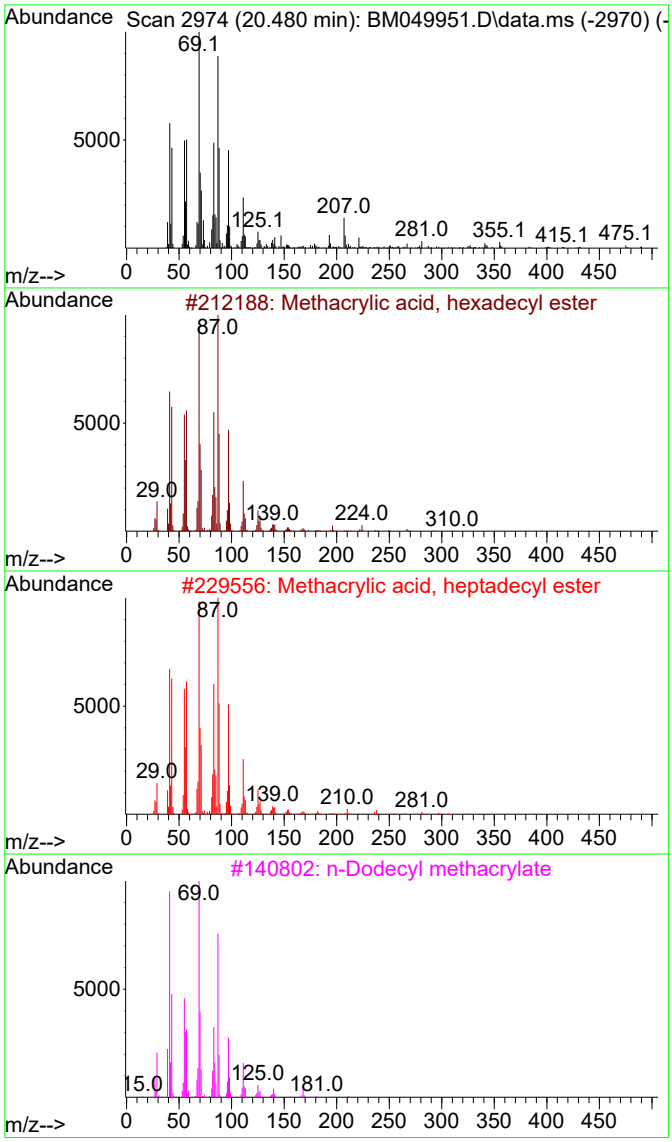
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

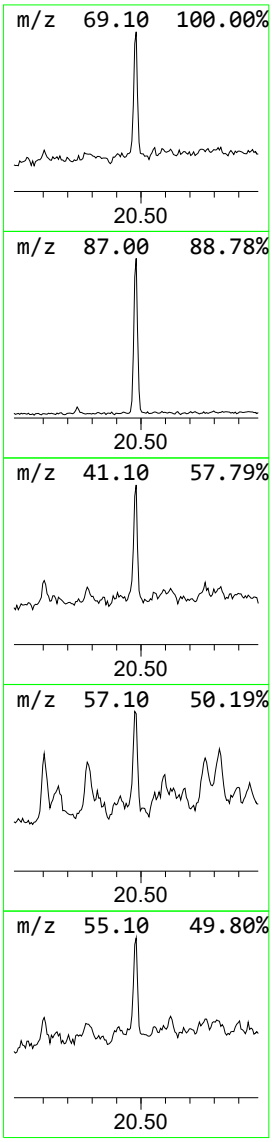
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Methacrylic acid, hexadecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.480	3.79 ng	604908	Chrysene-d12	21.397

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methacrylic acid, hexadecyl ester	310	C20H38O2	1000340-29-2	92
2	Methacrylic acid, heptadecyl ester	324	C21H40O2	1010340-29-3	70
3	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	68
4	Methacrylic acid, nonadecyl ester	352	C23H44O2	1000340-29-5	62
5	Octadecyl methacrylate	338	C22H42O2	000112-08-3	58





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Misc :
ALS Vial : 9 Sample Multiplier: 1

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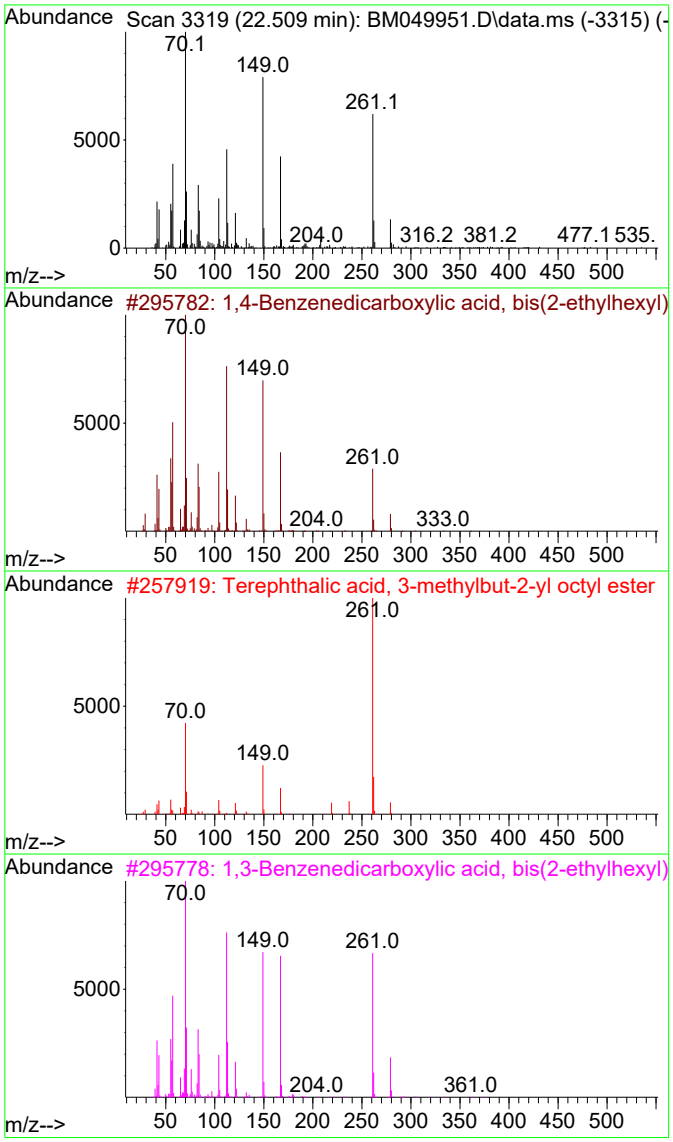
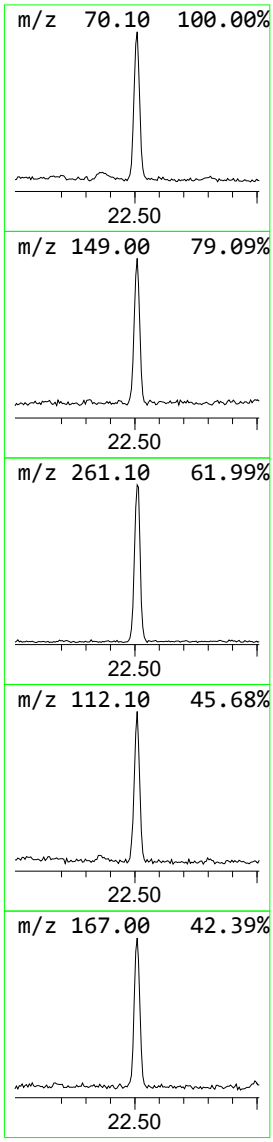
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1,4-Benzenedicarboxylic aci... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.509	3.22 ng	513170	Chrysene-d12	21.397

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	58
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
4	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	38
5	Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	27





Tentatively Identified Compound (LSC) summary

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Data File : BM049951.D
Acq On : 16 Apr 2025 14:07
Operator : RC/JU
Sample : Q1791-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
279312

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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
4-Penten-2-one,...	3.681	10.3	ng	1283090	1	7.769	2493990	20.0
3-Penten-2-one,...	4.287	134.0	ng	16712100	1	7.769	2493990	20.0
Cyclotrisiloxan...	4.416	77.4	ng	9653240	1	7.769	2493990	20.0
Furfural	4.787	2.3	ng	280658	1	7.769	2493990	20.0
Octane, 2,2,6-t...	8.445	2.1	ng	261494	1	7.769	2493990	20.0
Levoglucosenone	9.263	7.0	ng	1095050	2	10.563	3123360	20.0
Cyclopentasilox...	9.363	15.8	ng	2467400	2	10.563	3123360	20.0
Cyclohexasiloxa...	11.857	7.9	ng	1239690	2	10.563	3123360	20.0
Cycloheptasilox...	13.851	2.6	ng	328895	3	14.416	2558180	20.0
m-Cymene, 5-ter...	14.986	6.8	ng	870226	3	14.416	2558180	20.0
1H-Pyrrolo[3,2-...	15.174	3.3	ng	417512	3	14.416	2558180	20.0
n-Hexadecanoic ...	18.062	29.1	ng	6945610	4	17.157	4766500	20.0
Octadecanoic acid	19.339	13.1	ng	2081530	5	21.397	3189200	20.0
Methacrylic aci...	20.480	3.8	ng	604908	5	21.397	3189200	20.0
1,4-Benzenedica...	22.509	3.2	ng	513170	5	21.397	3189200	20.0