LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055196.D
Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-8-101322

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_G\Methods\8270-BG101322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.318	3	5	12	rVB	521570	671759	29.41%	6.432%
2	5.345	342	350	361	rBV	39813	69146	3.03%	0.662%
3	5.821	425	431	446	rBV	192430	330377	14.46%	3.163%
4	7.437	699	706	714	rBV	118909	215163	9.42%	2.060%
5	8.301	844	853	860	rBV	87885	152849	6.69%	1.463%
6	9.470	1045	1052	1060	rBV	331511	598470	26.20%	5.730%
7	9.558	1060	1067	1073	rVB	19032	33762	1.48%	0.323%
8	9.729	1089	1096	1103	rVB	17240	29173	1.28%	0.279%
9	9.928	1123	1130	1141	rBV	68081	149961	6.57%	1.436%
10	11.133	1328	1335	1350	rVB	129899	239945	10.50%	2.297%
11	12.508	1560	1569	1575	rVB6	19773	45754	2.00%	0.438%
12	12.790	1612	1617	1627	rVB4	15981	33775	1.48%	0.323%
13	13.542	1735	1745	1754	rBV	985489	1539073	67.38%	14.736%
14	13.747	1773	1780	1783	rBV	97609	155894	6.82%	1.493%
15	13.789	1783	1787	1794	rVB	85219	135528	5.93%	1.298%
16	13.959	1811	1816	1822	rBV2	18495	29072	1.27%	0.278%
17	14.423	1891	1895	1903	rBV8	16657	26863	1.18%	0.257%
18	14.752	1946	1951	1958	rVB2	41839	72956	3.19%	0.699%
19	14.911	1969	1978	1986	rBV	225805	373930	16.37%	3.580%
20	15.169	2018	2022	2030	rVB6	15497	23289	1.02%	0.223%
21	15.522	2078	2082	2088	rVB	16317	26072	1.14%	0.250%
22	16.080	2173	2177	2181	rVB	31020	39826	1.74%	0.381%
23	16.385	2223	2229	2238	rVB	869629	1334888	58.44%	12.781%
24	16.562	2255	2259	2264	rBV3	22141	34391	1.51%	0.329%
25	17.373	2394	2397	2401	rBV4	17211	23845	1.04%	0.228%
26	17.643	2437	2443	2449	rBV	312229	459859	20.13%	4.403%
27	18.289	2549	2553	2557	rVB3	41635	56908	2.49%	0.545%
28	18.495	2584	2588	2598	rBV3	52816	95439	4.18%	0.914%
29	19.541	2763	2766	2771	rVB	21315	29475	1.29%	0.282%
30	19.752	2798	2802	2814	rVB3	46407	93690	4.10%	0.897%
31	20.028	2846	2849	2854	rVB2	19566	24697	1.08%	0.236%
32	20.222	2876	2882	2888	rBV	1709870	2284247	100.00%	21.871%
33	21.926	3166	3172	3180	rVB2	275059	490349	21.47%	4.695%
34	25.351	3746	3755	3766	rVB2	171097	523664	22.93%	5.014%

Sum of corrected areas: 10444089

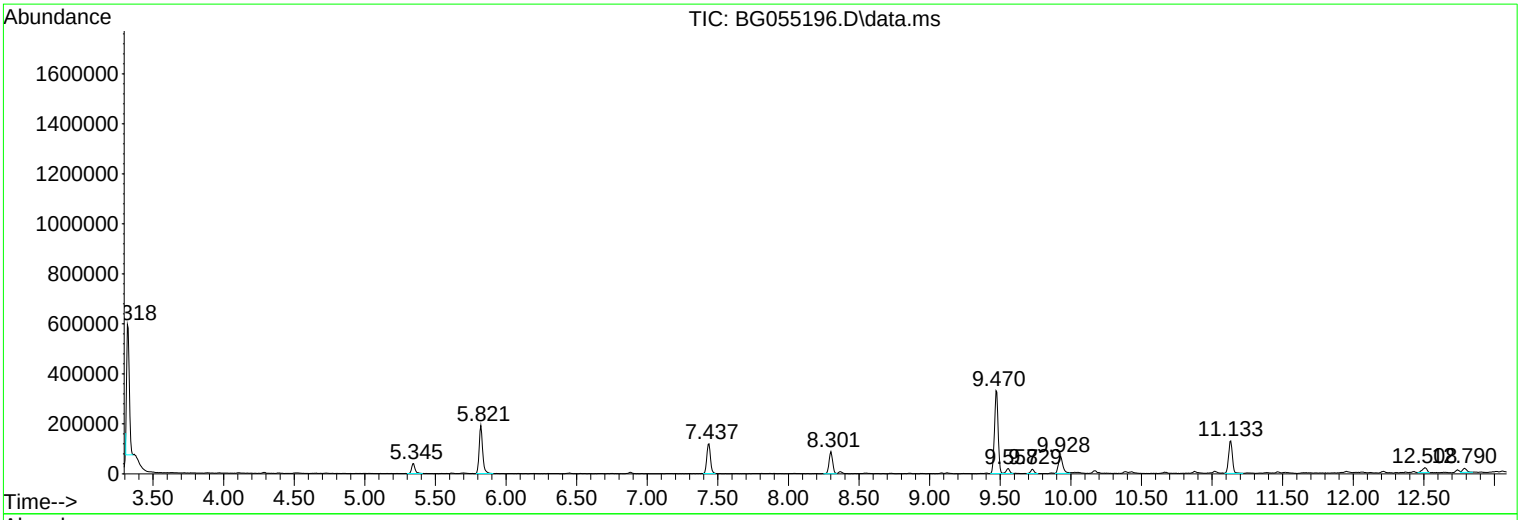
Instrument :
BNA_G
ClientSampleId :
MW-8-101322

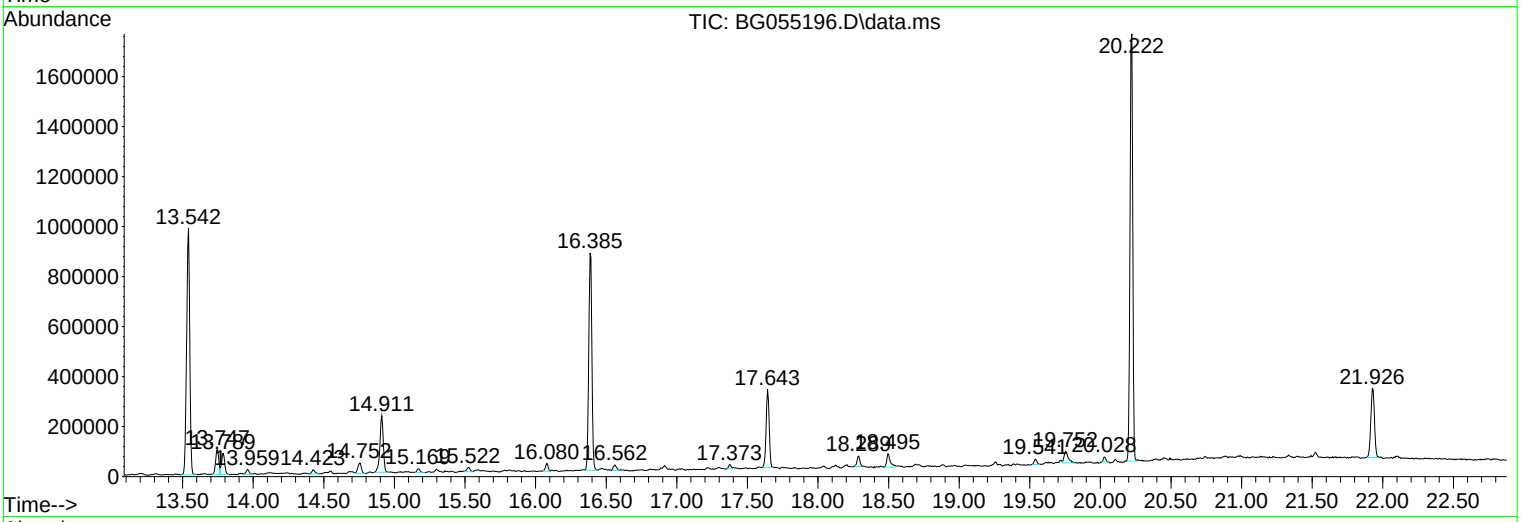
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055196.D
Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

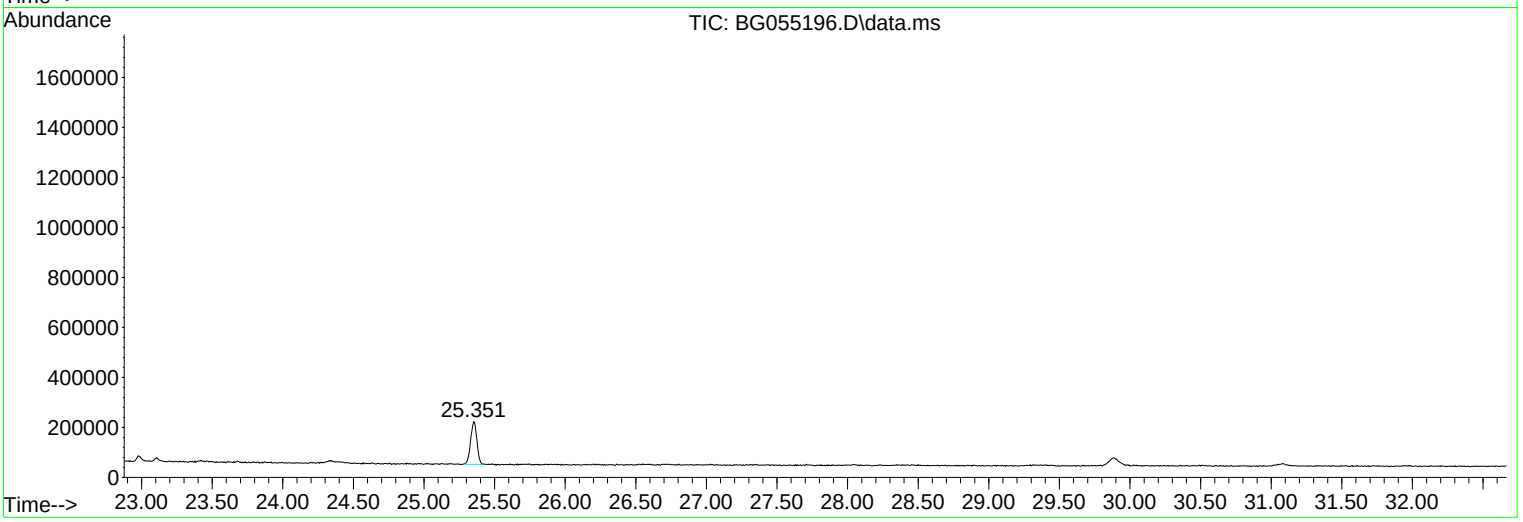
Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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TIC Library : C:\Database\NIST20.L
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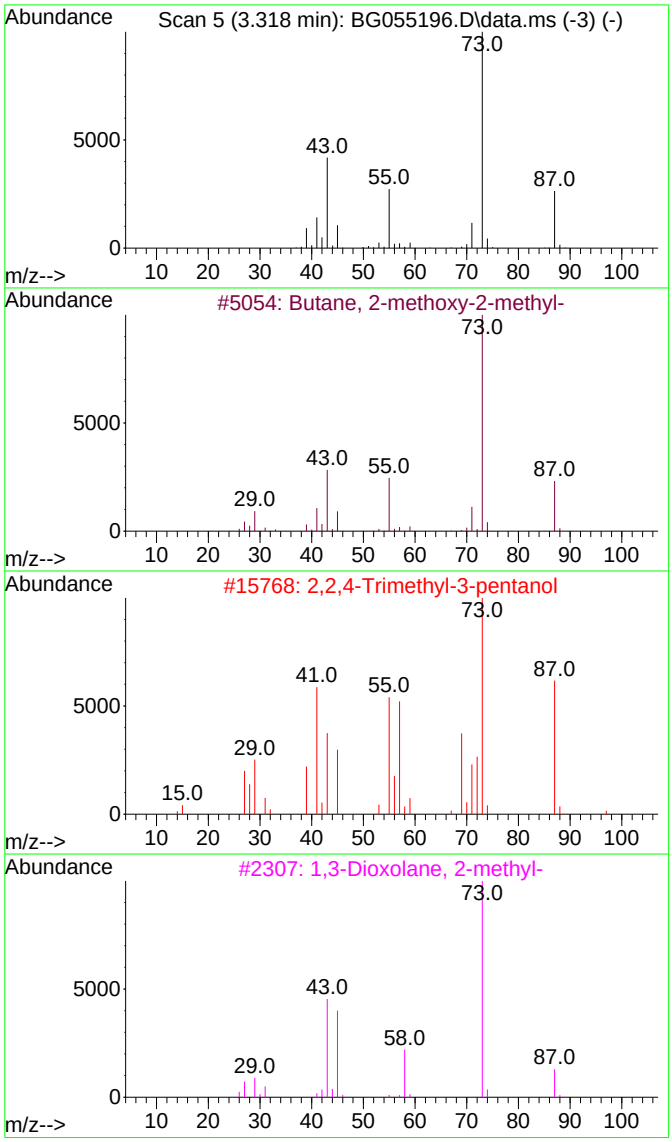
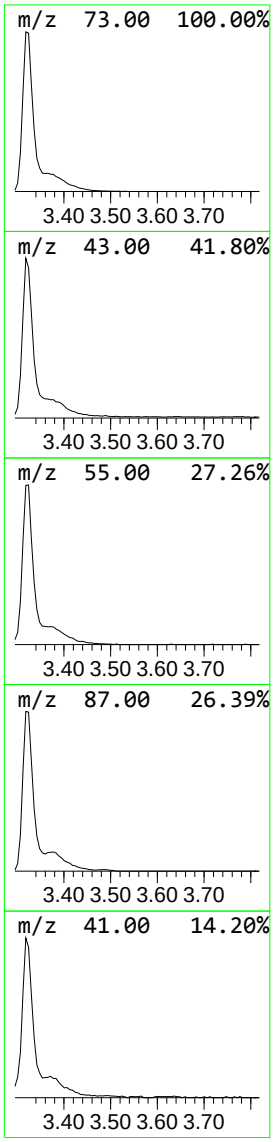
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.318	87.90 ng	671759	1,4-Dichlorobenzene-d4	8.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-8-101322

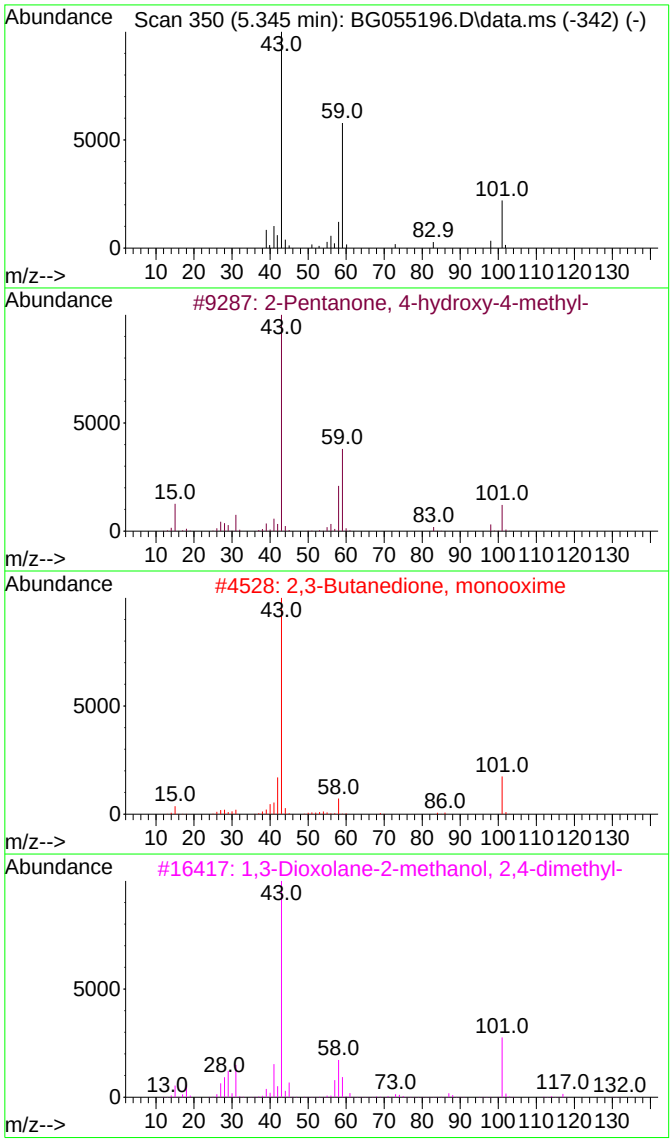
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

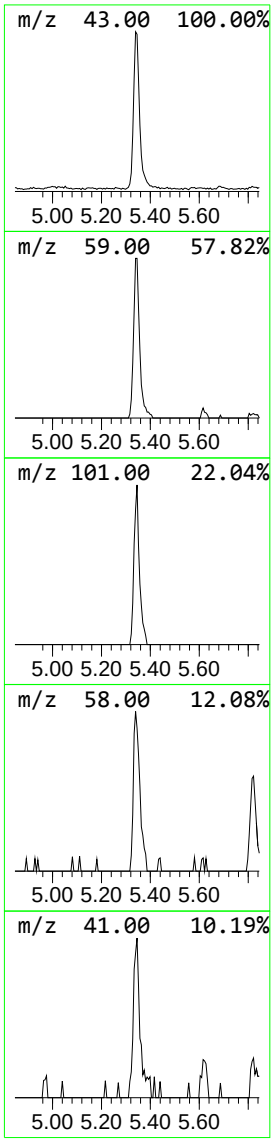
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.345	9.05 ng	69146	1,4-Dichlorobenzene-d4	8.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
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TIC Library : C:\Database\NIST20.L
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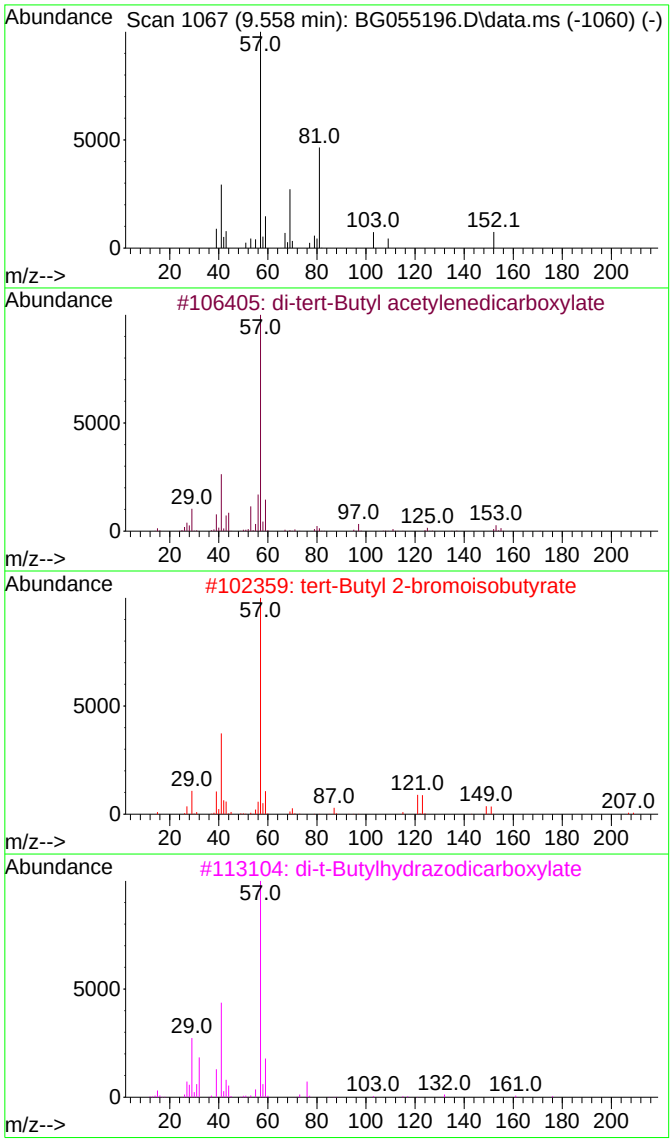
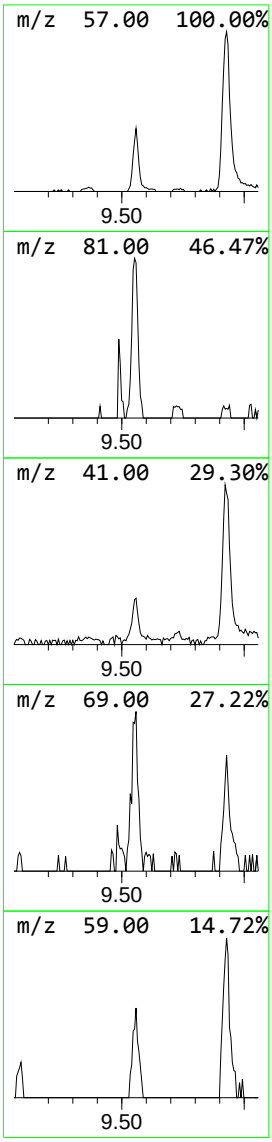
****

Peak Number 3 unknown9.558 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.558	4.42 ng	33762	1,4-Dichlorobenzene-d4	8.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	32
2	tert-Butyl 2-bromoisobutyrate	222	C8H15BrO2	023877-12-5	16
3	di-t-Butylhydrazodicarboxylate	232	C10H20N2O4	016466-61-8	12
4	1,5-Pentanediol, O,O'-dipivaloyl-	272	C15H28O4	1000330-92-4	10
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	9





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Sample : N5145-05
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Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
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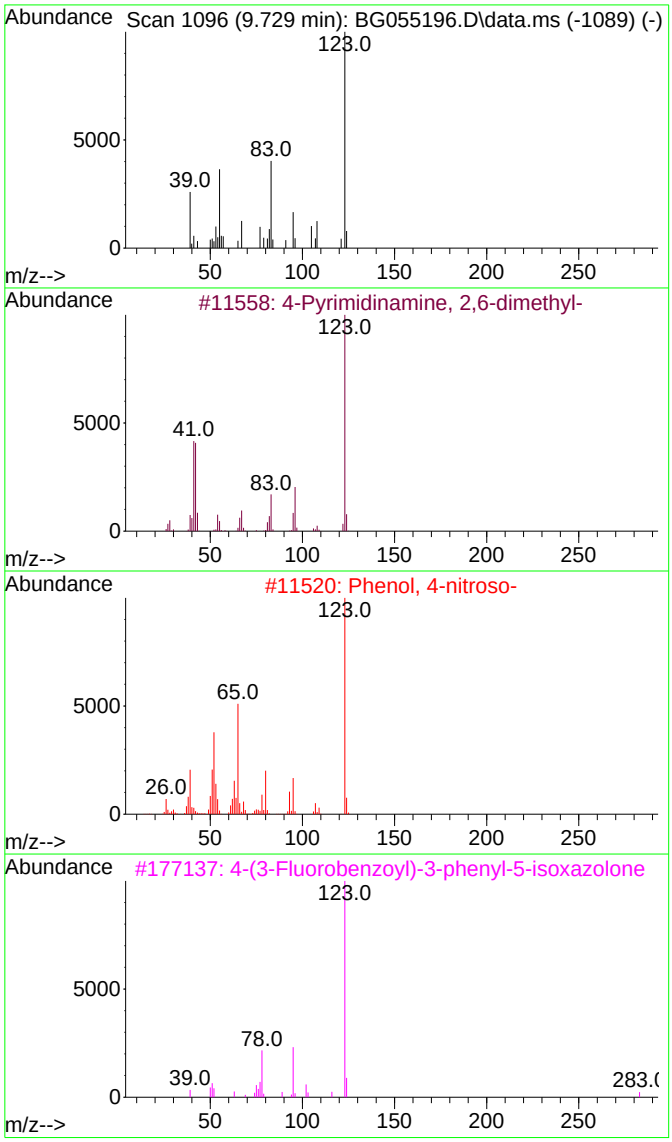
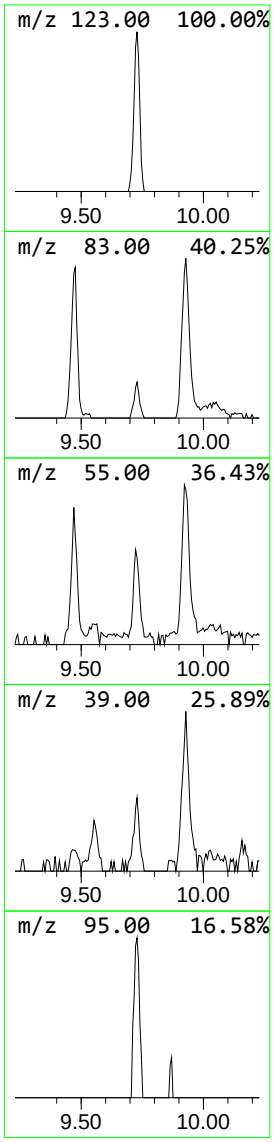
****

Peak Number 4 unknown9.729 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.729	2.43 ng	29173	Naphthalene-d8	11.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	47
2	Phenol, 4-nitroso-	123	C6H5NO2	000104-91-6	43
3	4-(3-Fluorobenzoyl)-3-phenyl-5-i...	283	C16H10FNO3	1000434-46-1	43
4	3-Pyridinol, 2,6-dimethyl-	123	C7H9NO	001122-43-6	43
5	1H-Tetraazol-5-ylacetonitrile, N...	123	C4H5N5	1344273-80-8	43





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Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

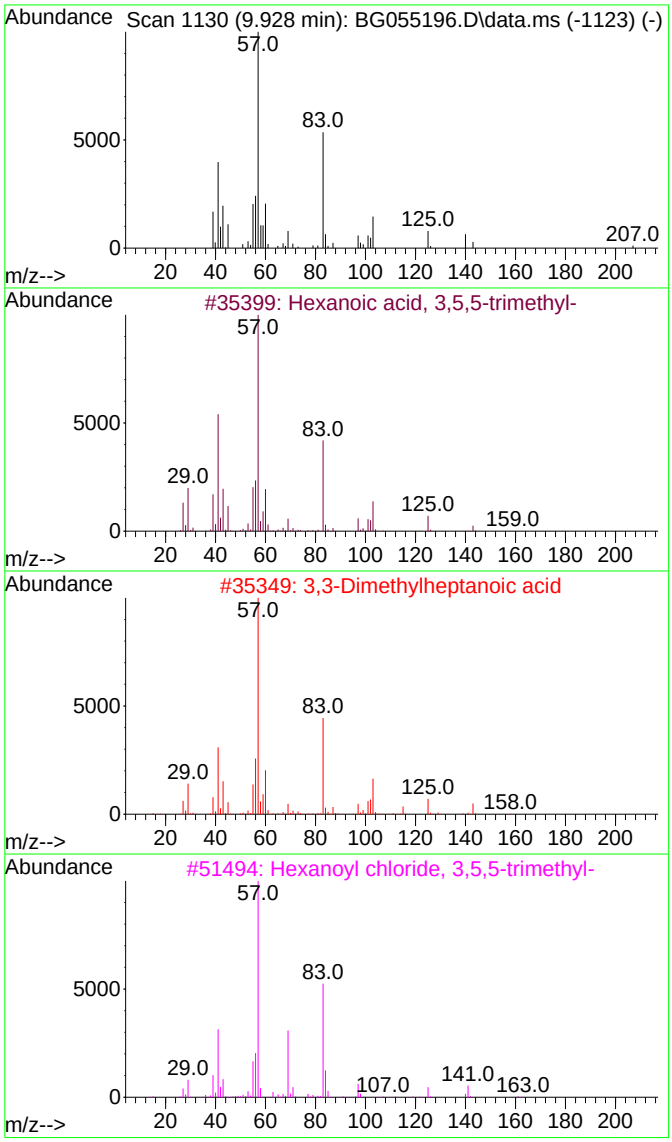
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

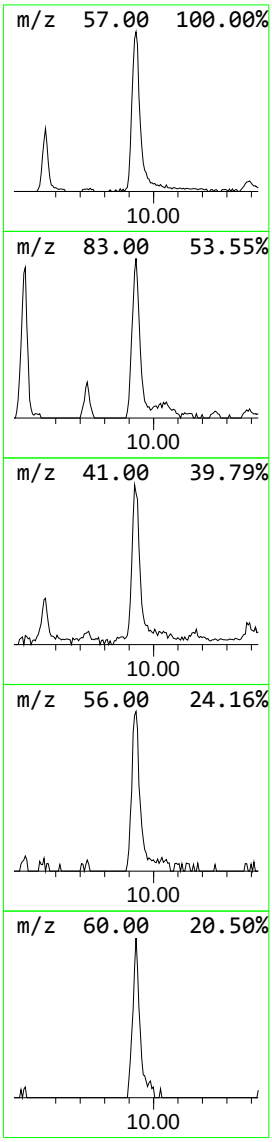
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanoic acid, 3,5,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.928	12.50 ng	149961	Naphthalene-d8	11.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	78
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	38
4	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	38
5	Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	27





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Instrument :
BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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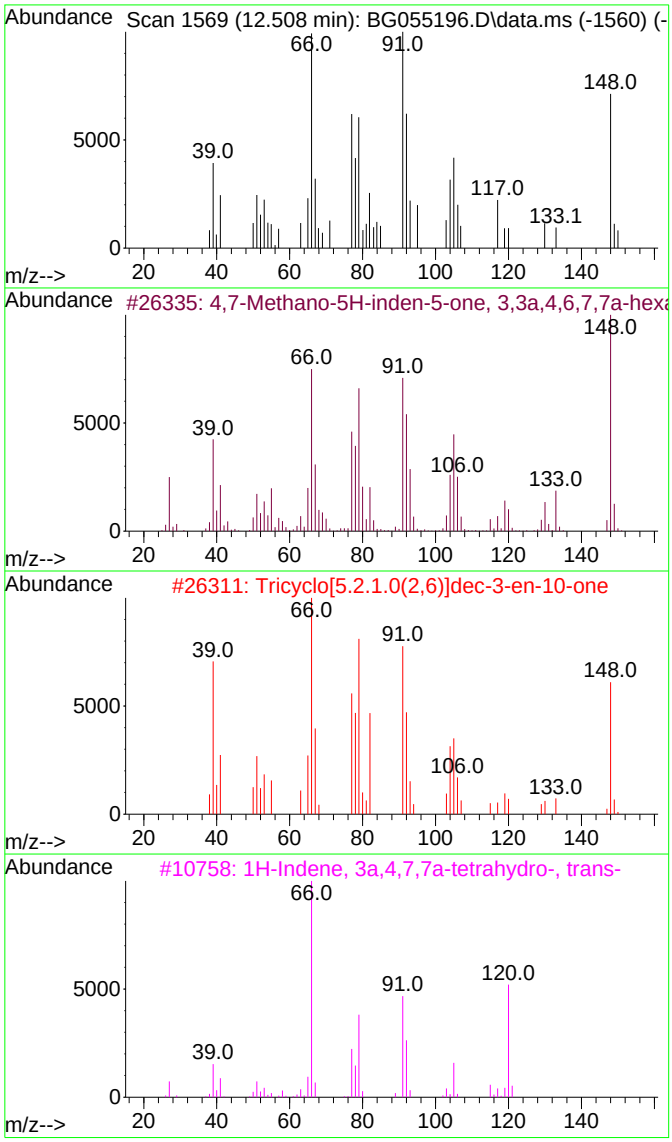
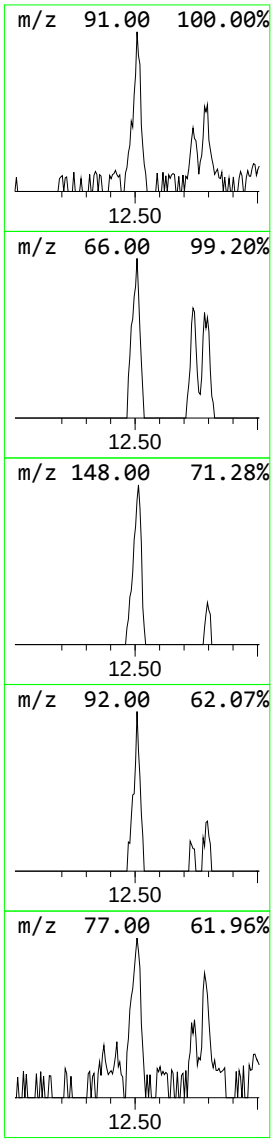
****
Peak Number 6 4,7-Methano-5H-inden-5-one,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.508	3.81 ng	45754	Naphthalene-d8	11.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	91
2	Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	91
3	1H-Indene, 3a,4,7,7a-tetrahydro-...	120	C9H12	066563-20-0	59
4	exo-Norborneol, trifluoroacetate	208	C9H11F3O2	031024-13-2	50
5	4-Nonen-2-yne, (E)-	122	C9H14	053497-79-3	50





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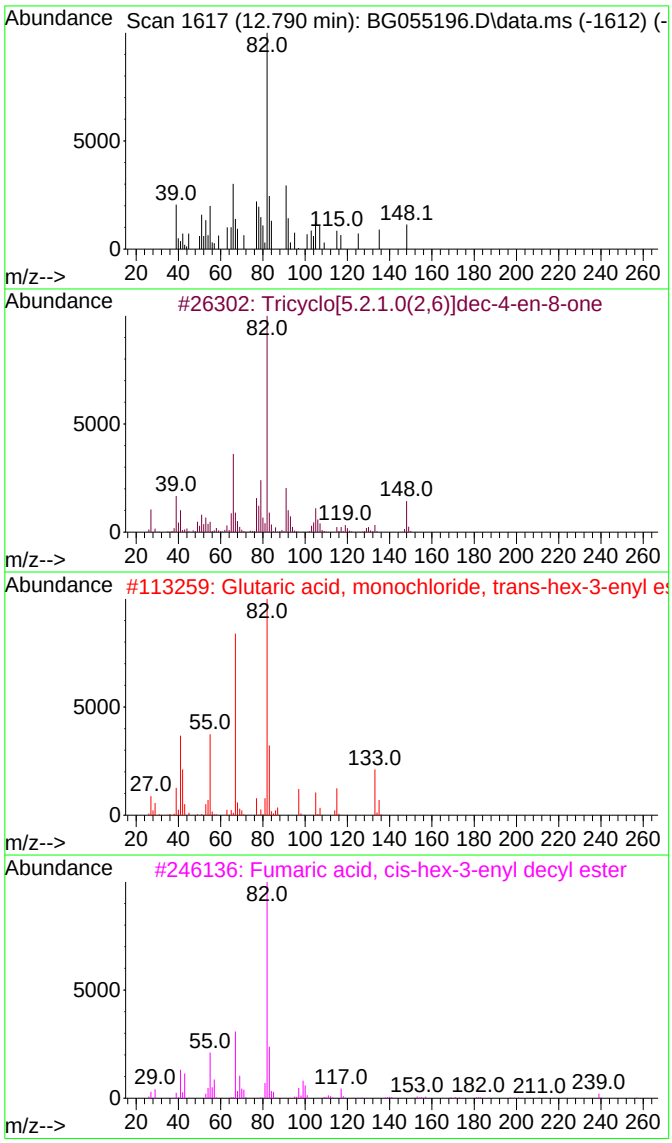
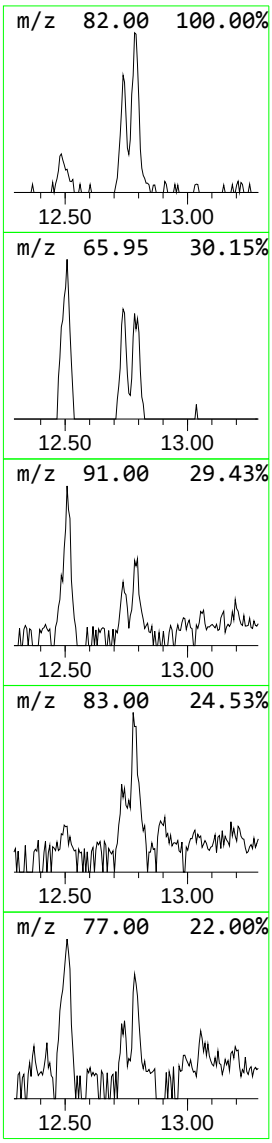
****
Peak Number 7 Tricyclo[5.2.1.0(2,6)]dec-4... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.790	2.82 ng	33775	Naphthalene-d8	11.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.1.0(2,6)]dec-4-en-8...	148	C10H12O	1000191-39-7	72
2	Glutaric acid, monochloride, tra...	232	C11H17ClO3	1000359-93-9	12
3	Fumaric acid, cis-hex-3-enyl dec...	338	C20H34O4	1010348-86-6	10
4	Fumaric acid, cis-hex-3-enyl non...	324	C19H32O4	1000348-86-5	10
5	Methanamine, N-[3-methyl-2-buten...	97	C6H11N	1000196-86-4	10





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TIC Library : C:\Database\NIST20.L
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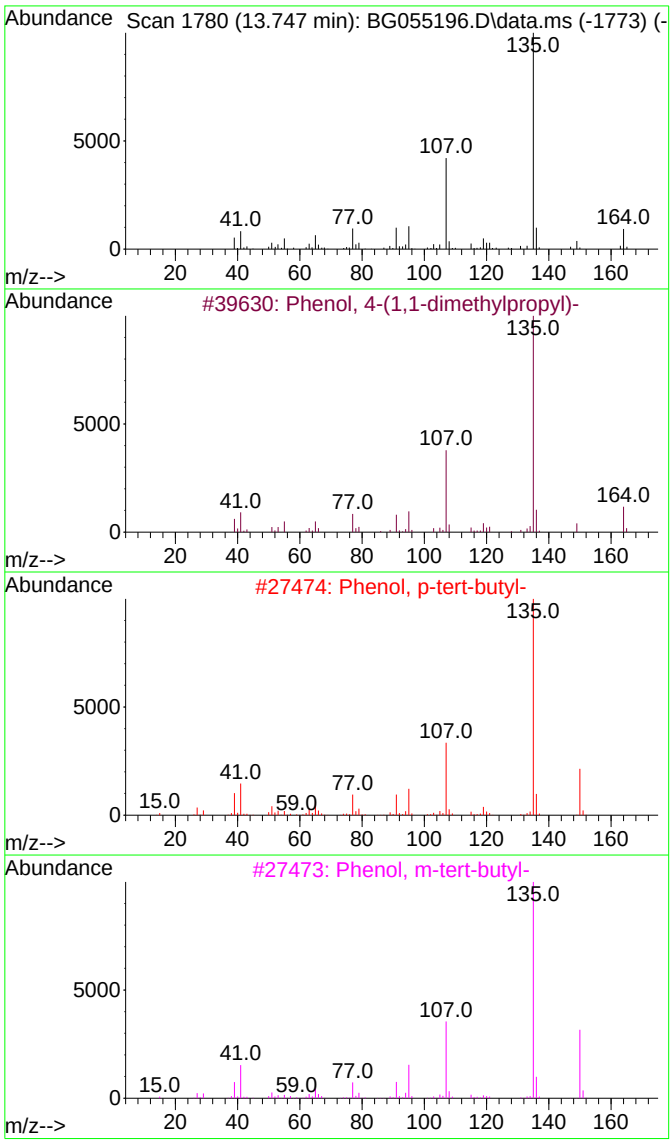
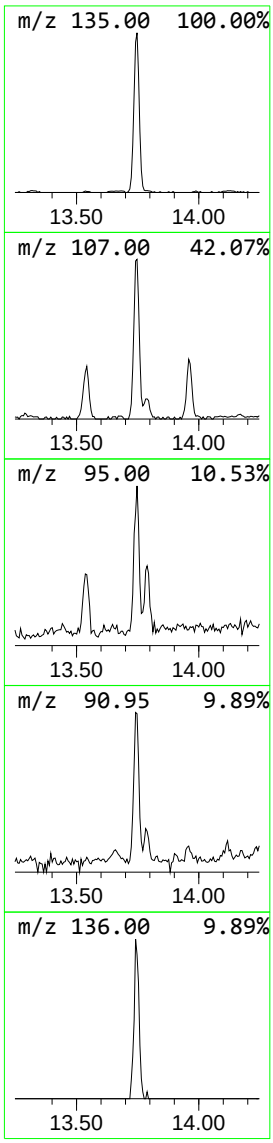
****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.747	8.34 ng	155894	Acenaphthene-d10	14.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64





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TIC Integration Parameters: LSCINT.P

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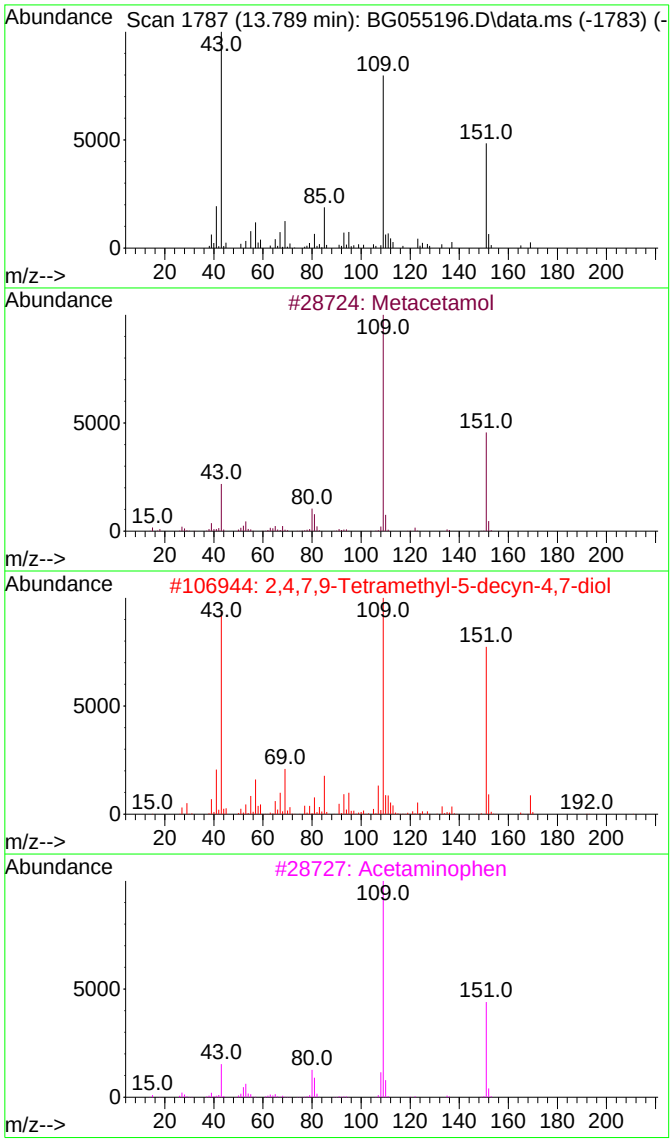
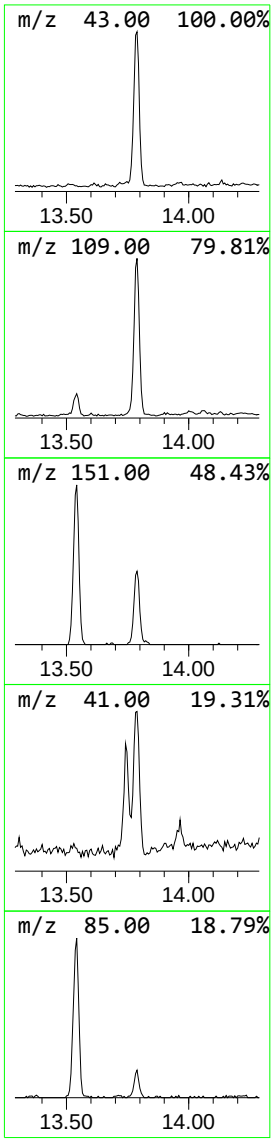
Peak Number 9 Metacetamol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.789	7.25 ng	135528	Acenaphthene-d10	14.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	59
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	50
3	Acetaminophen	151	C8H9NO2	000103-90-2	45
4	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	45
5	4-Amino-2-methylpyrimidine	109	C5H7N3	000074-69-1	43





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Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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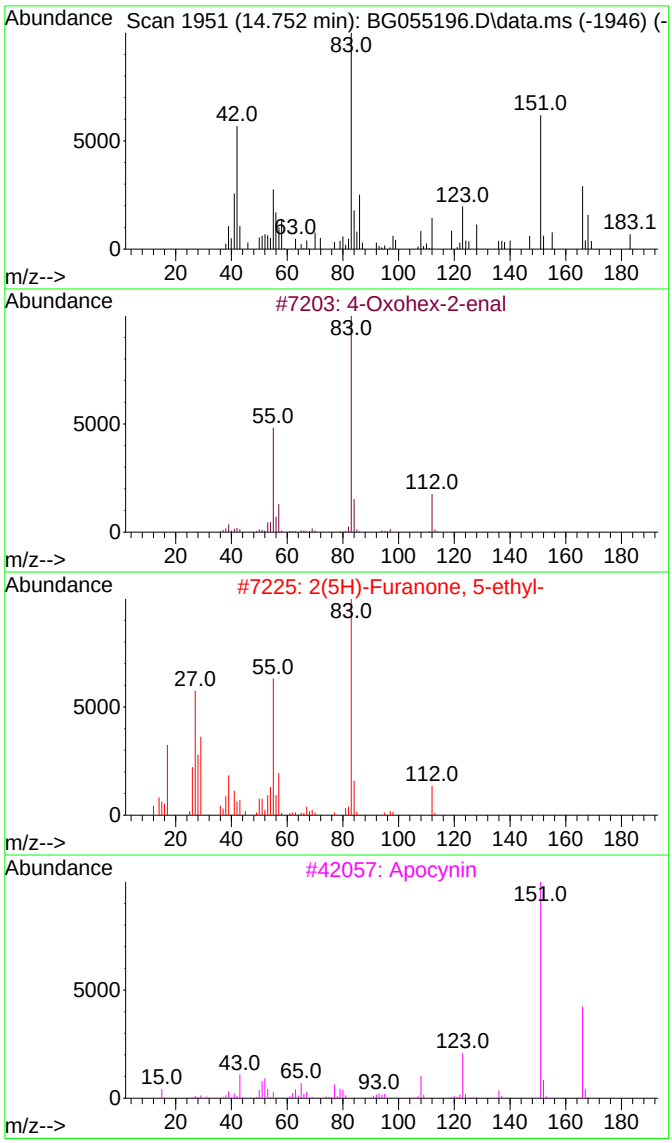
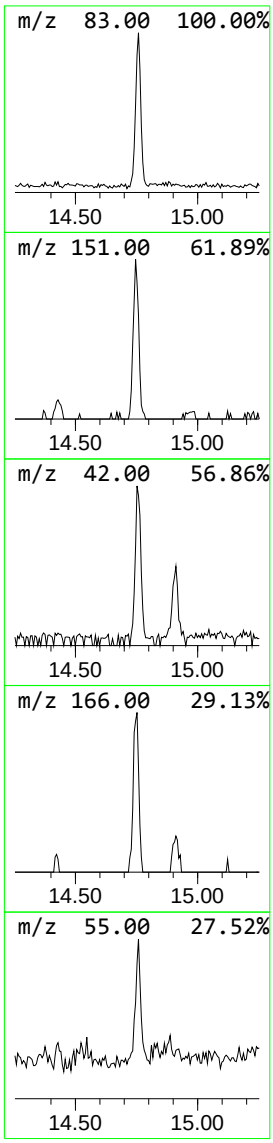
Peak Number 10 unknown14.752 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.752	3.90 ng	72956	Acenaphthene-d10	14.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Oxohex-2-enal	112	C6H8O2	020697-55-6	22
2	2(5H)-Furanone, 5-ethyl-	112	C6H8O2	002407-43-4	22
3	Apocynin	166	C9H10O3	000498-02-2	20
4	But-2-enoic acid, amide, 3-methy...	139	C8H13NO	1000340-08-9	14
5	t-Butylhydroquinone	166	C10H14O2	001948-33-0	14





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Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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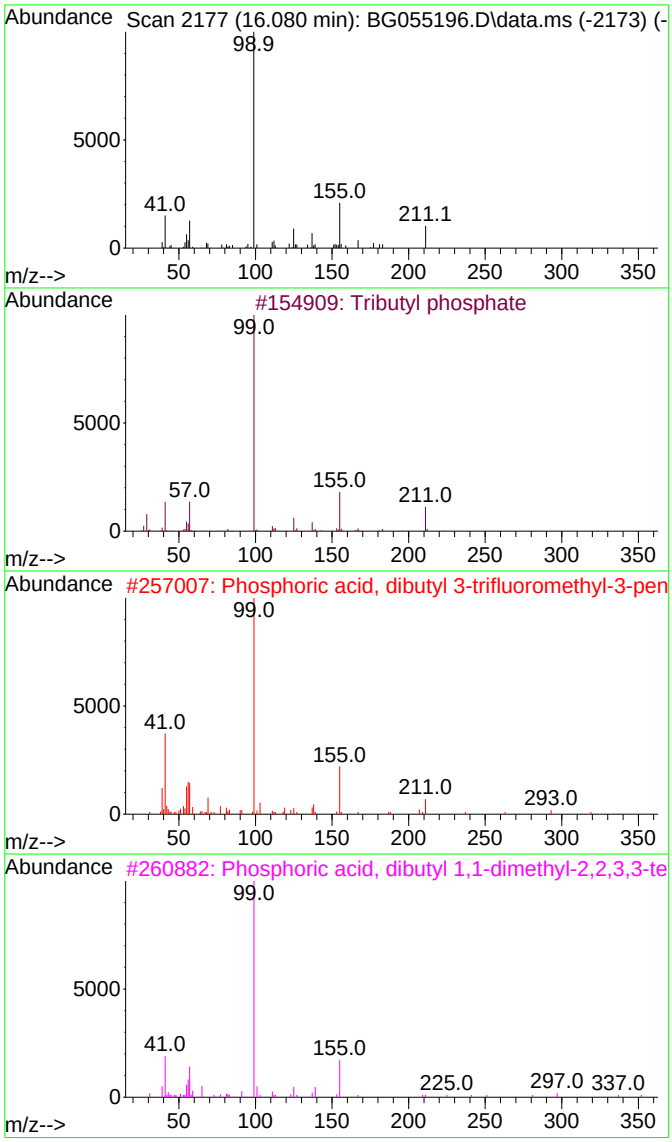
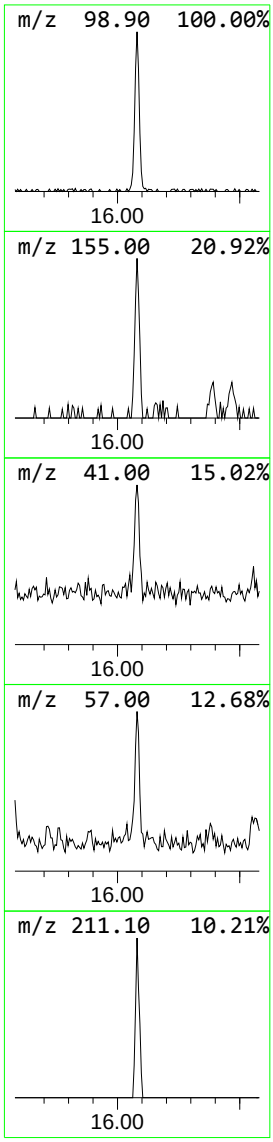
Peak Number 11 Tributyl phosphate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	2.13 ng	39826	Acenaphthene-d10	14.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	90
2	Phosphoric acid, dibutyl 3-trifl...	348	C14H28F3O4P	1000298-93-8	72
3	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	50
4	7-Methylhexahydrocyclopenta[c]py...	154	C9H14O2	091108-59-7	43
5	1,4-Dioxaspiro[4.6]undec-7-ene	154	C9H14O2	007140-60-5	38





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Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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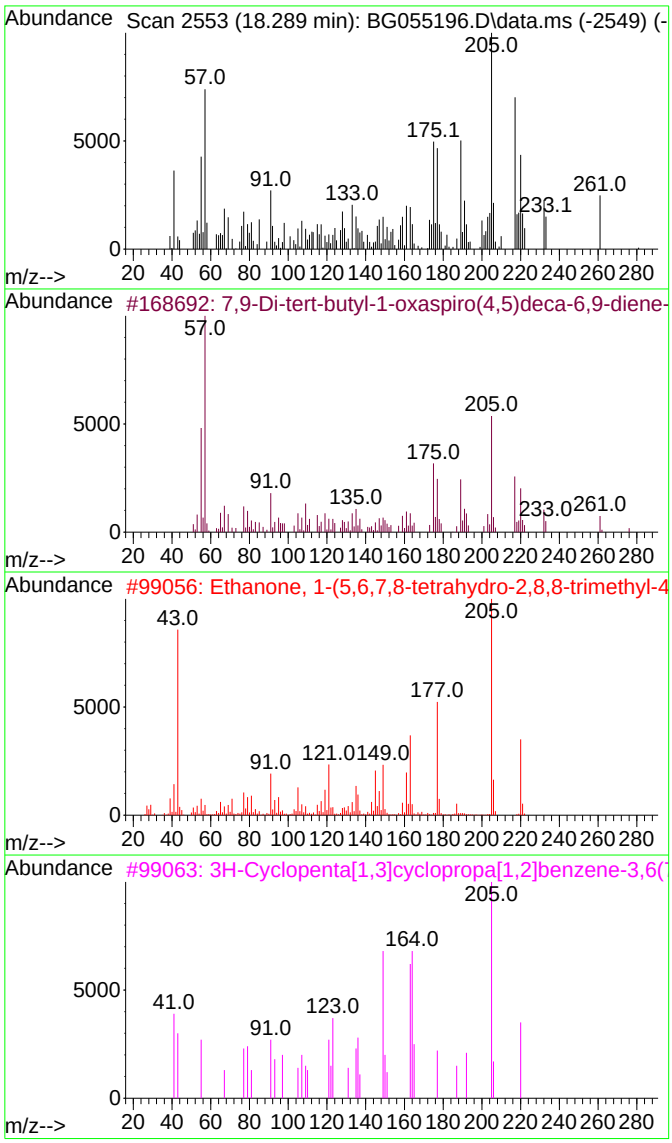
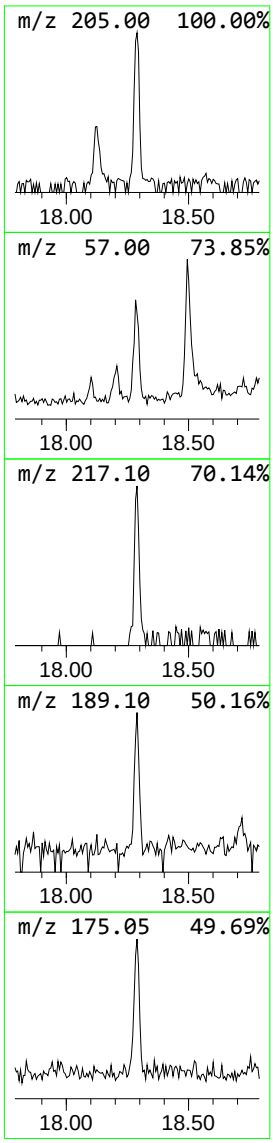
Peak Number 12 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.289	2.48 ng	56908	Phenanthrene-d10	17.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	38
4	2H-2a,7-Methanoazuleno[5,6-b]oxi...	220	C15H24O	029597-36-2	30
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	30





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Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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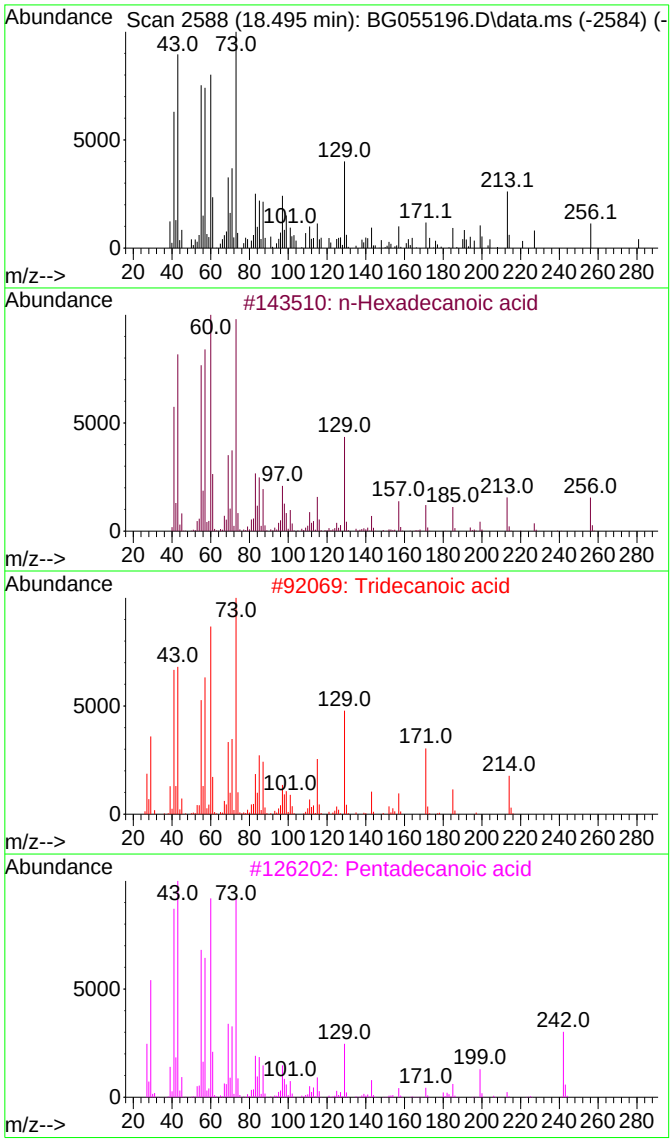
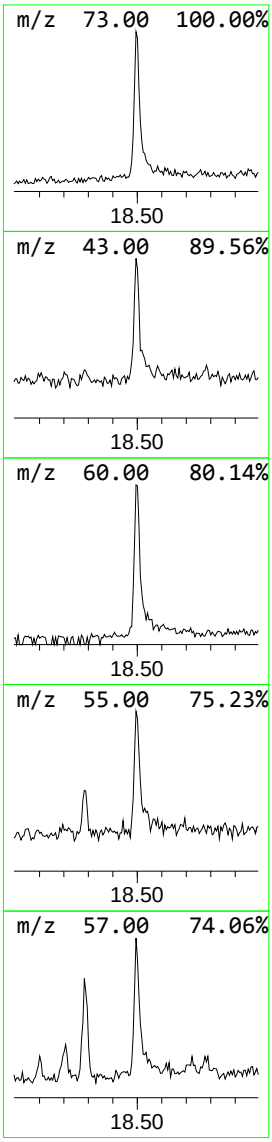
Peak Number 13 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.495	4.15 ng	95439	Phenanthrene-d10	17.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055196.D
Acq On : 17 Oct 2022 17:22
Operator : CG/JU
Sample : N5145-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-8-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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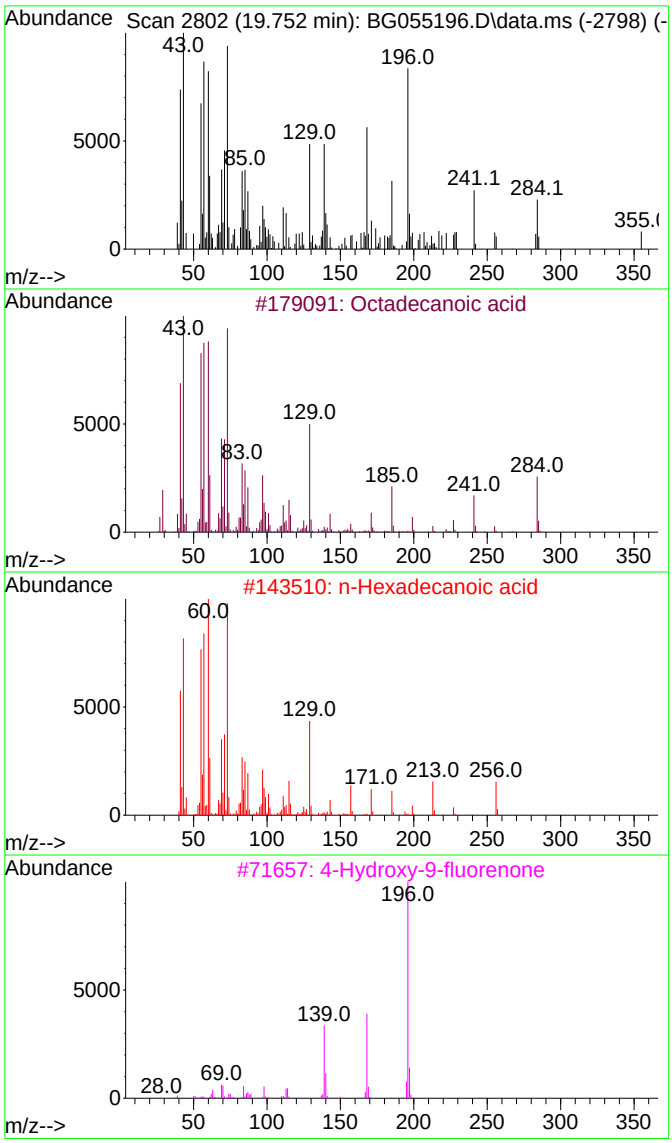
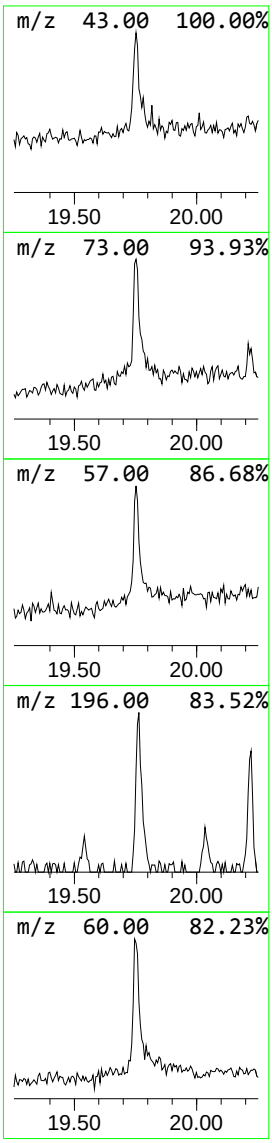
Peak Number 14 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.752	4.07 ng	93690	Phenanthrene-d10	17.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
3	4-Hydroxy-9-fluorenone	196	C13H8O2	001986-00-1	42
4	Xanthone	196	C13H8O2	000090-47-1	42
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	42





Tentatively Identified Compound (LSC) summary

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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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
Butane, 2-metho...	3.318	87.9	ng	671759	1	8.301	152849	20.0
2-Pentanone, 4-...	5.345	9.1	ng	69146	1	8.301	152849	20.0
unknown9.558	9.558	4.4	ng	33762	1	8.301	152849	20.0
unknown9.729	9.729	2.4	ng	29173	2	11.133	239945	20.0
Hexanoic acid, ...	9.928	12.5	ng	149961	2	11.133	239945	20.0
4,7-Methano-5H-...	12.508	3.8	ng	45754	2	11.133	239945	20.0
Tricyclo[5.2.1....	12.790	2.8	ng	33775	2	11.133	239945	20.0
Phenol, 4-(1,1-...	13.747	8.3	ng	155894	3	14.911	373930	20.0
Metacetamol	13.789	7.3	ng	135528	3	14.911	373930	20.0
unknown14.752	14.752	3.9	ng	72956	3	14.911	373930	20.0
Tributyl phosphate	16.080	2.1	ng	39826	3	14.911	373930	20.0
7,9-Di-tert-but...	18.289	2.5	ng	56908	4	17.643	459859	20.0
n-Hexadecanoic ...	18.495	4.2	ng	95439	4	17.643	459859	20.0
Octadecanoic acid	19.752	4.1	ng	93690	4	17.643	459859	20.0