LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107543.D
Acq On : 21 Jul 2018 00:03
Operator : JU/SJ
Sample : J4018-02 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

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_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.607	552	556	570	rBV2	71908	226568	3.58%	0.866%
2	6.613	722	727	745	rBV2	63059	210225	3.32%	0.804%
3	6.742	746	749	765	rBV	392534	646184	10.21%	2.471%
4	6.972	784	788	808	rBV	1574569	1816612	28.71%	6.947%
5	7.125	810	814	833	rVB	582518	696437	11.01%	2.663%
6	7.536	880	884	899	rBV	317332	532333	8.41%	2.036%
7	8.060	965	973	979	rBV	207592	314647	4.97%	1.203%
8	8.142	979	987	988	rVV	259843	374360	5.92%	1.432%
9	8.160	988	990	993	rVV	240487	275645	4.36%	1.054%
10	8.189	993	995	1000	rVB4	99319	115030	1.82%	0.440%
11	8.254	1002	1006	1016	rBV	2253443	2323430	36.72%	8.885%
12	8.601	1060	1065	1068	rBV2	85431	116484	1.84%	0.445%
13	9.325	1184	1188	1203	rBV	1050605	1181413	18.67%	4.518%
14	9.436	1203	1207	1210	rBV	86181	84795	1.34%	0.324%
15	9.719	1252	1255	1259	rBV	154672	162946	2.58%	0.623%
16	10.013	1301	1305	1312	rBV	2348626	2462479	38.92%	9.417%
17	10.436	1371	1377	1380	rBV	6329200	6326848	100.00%	24.195%
18	10.807	1437	1440	1448	rBV	591609	603077	9.53%	2.306%
19	11.507	1555	1559	1567	rBV	2284696	2235387	35.33%	8.549%
20	12.018	1643	1646	1651	rBV	87518	113255	1.79%	0.433%
21	13.089	1825	1828	1833	rBV	892292	746356	11.80%	2.854%
22	14.159	2006	2010	2013	rVV	1939113	1922211	30.38%	7.351%
23	14.195	2013	2016	2020	rVB2	113766	122399	1.93%	0.468%
24	14.577	2079	2081	2084	rBV	95402	106282	1.68%	0.406%
25	14.977	2146	2149	2151	rBV	115937	149506	2.36%	0.572%
26	15.006	2151	2154	2158	rVB2	189248	231839	3.66%	0.887%
27	15.689	2265	2270	2276	rVB2	1529706	2052293	32.44%	7.848%

Sum of corrected areas: 26149041

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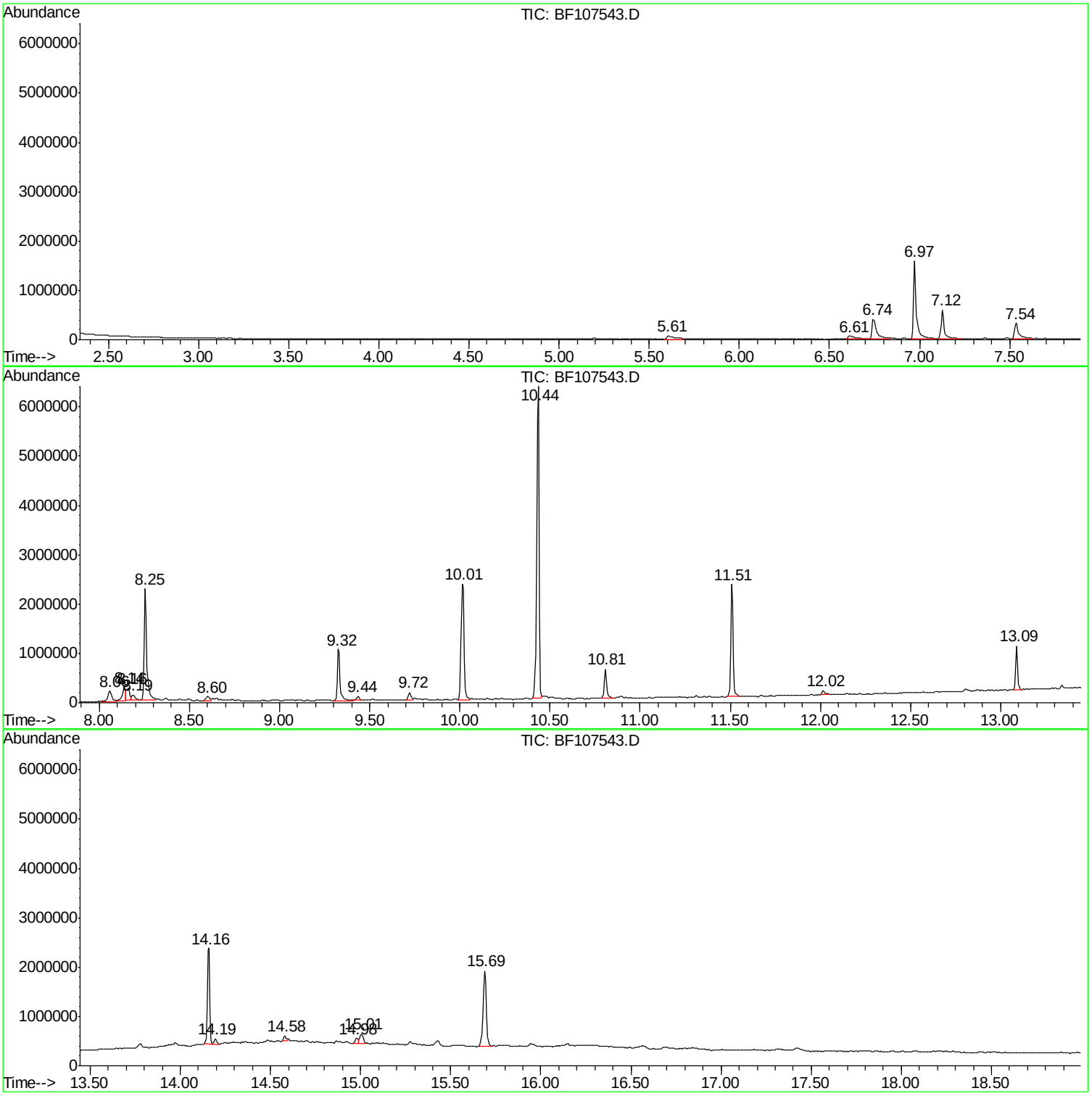
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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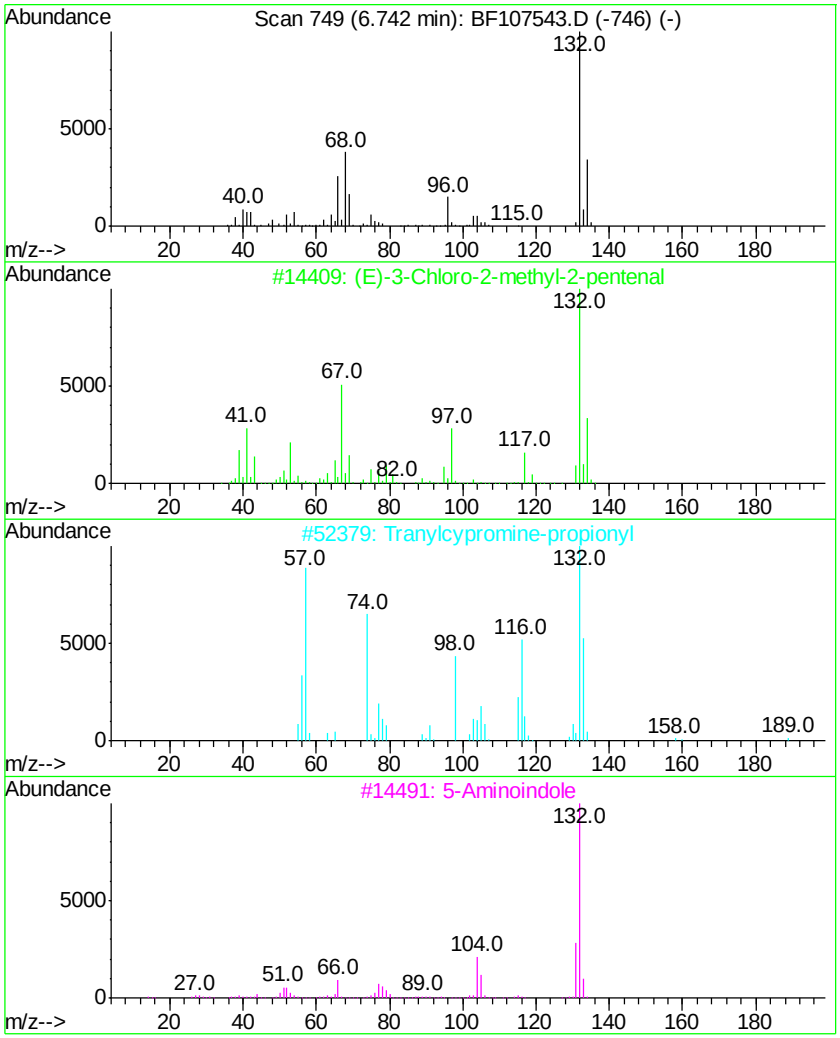
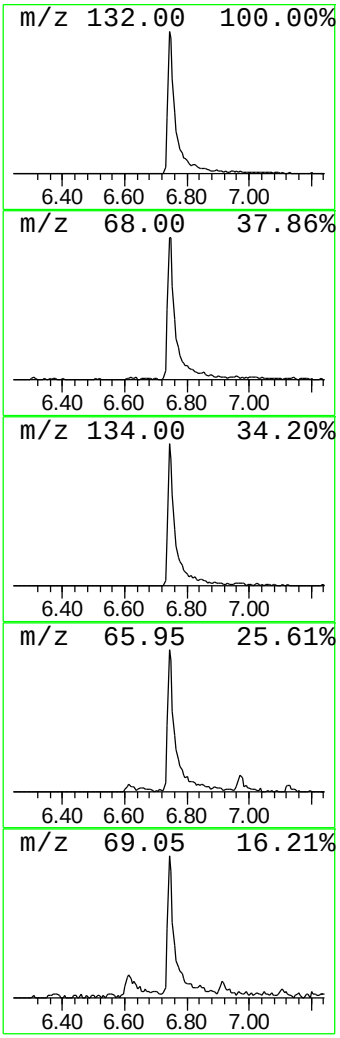
Peak Number 1 unknown6.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	7.11 ng	646184	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF107543.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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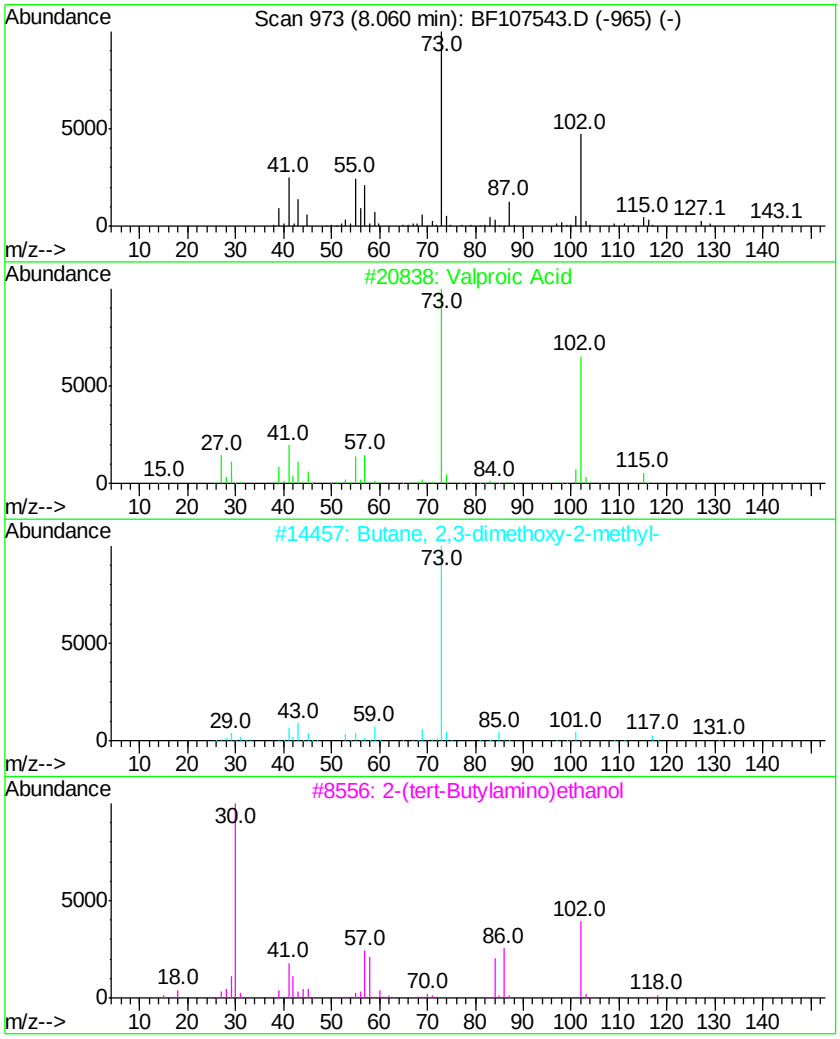
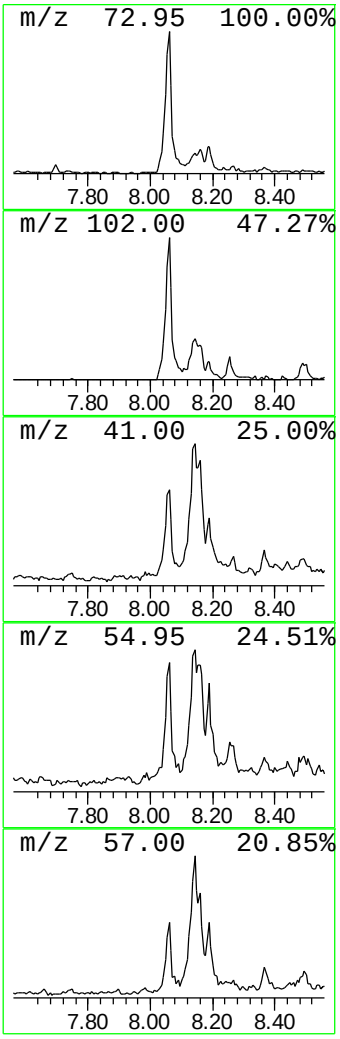
Peak Number 3 Valproic Acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	2.71 ng	314647	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valproic Acid	144	C8H16O2	000099-66-1	53
2	Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	10
3	2-(tert-Butylamino)ethanol	117	C6H15NO	004620-70-6	9
4	Neopentylamine	87	C5H13N	005813-64-9	9
5	3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107543.D
Acq On : 21 Jul 2018 00:03
Operator : JU/SJ
Sample : J4018-02 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

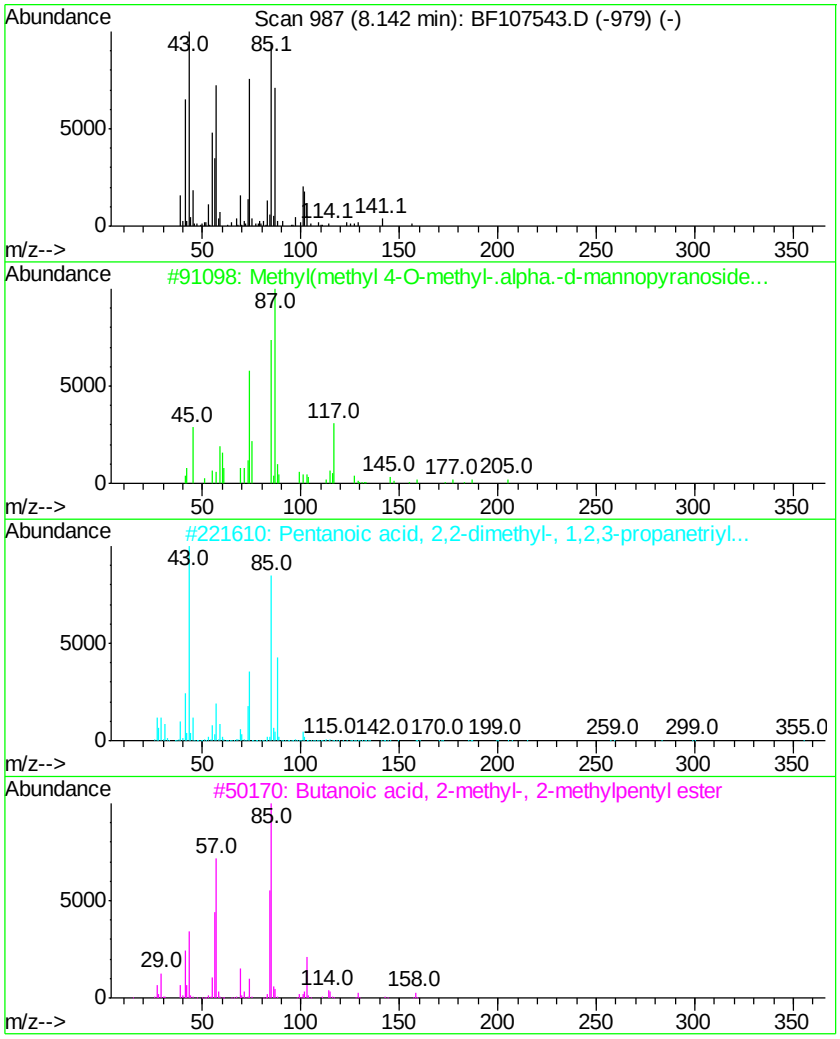
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

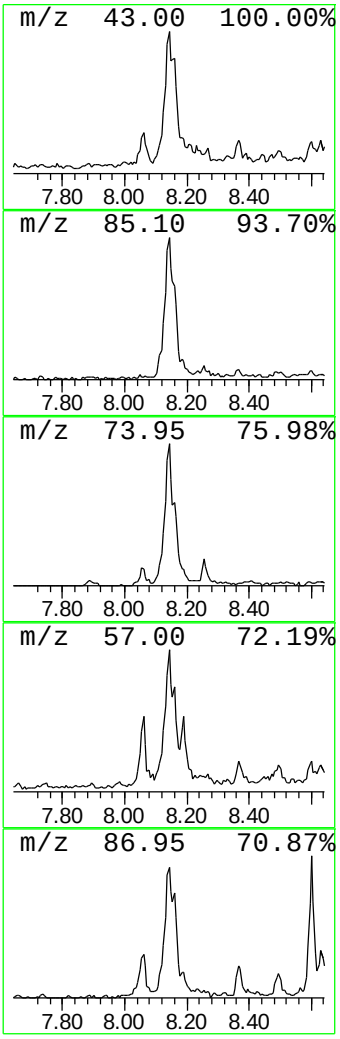
****

Peak Number 4 unknown8.14 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.14	3.22 ng	374360	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl(methyl 4-O-methyl-.alpha....	236	C9H16O7	024916-47-0	38
2	Pentanoic acid, 2,2-dimethyl-, 1...	428	C24H44O6	057346-62-0	35
3	Butanoic acid, 2-methyl-, 2-meth...	186	C11H22O2	083783-88-4	27
4	Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	22
5	Heptane, 2-(hexyloxy)-	200	C13H28O	074663-79-9	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107543.D
Acq On : 21 Jul 2018 00:03
Operator : JU/SJ
Sample : J4018-02 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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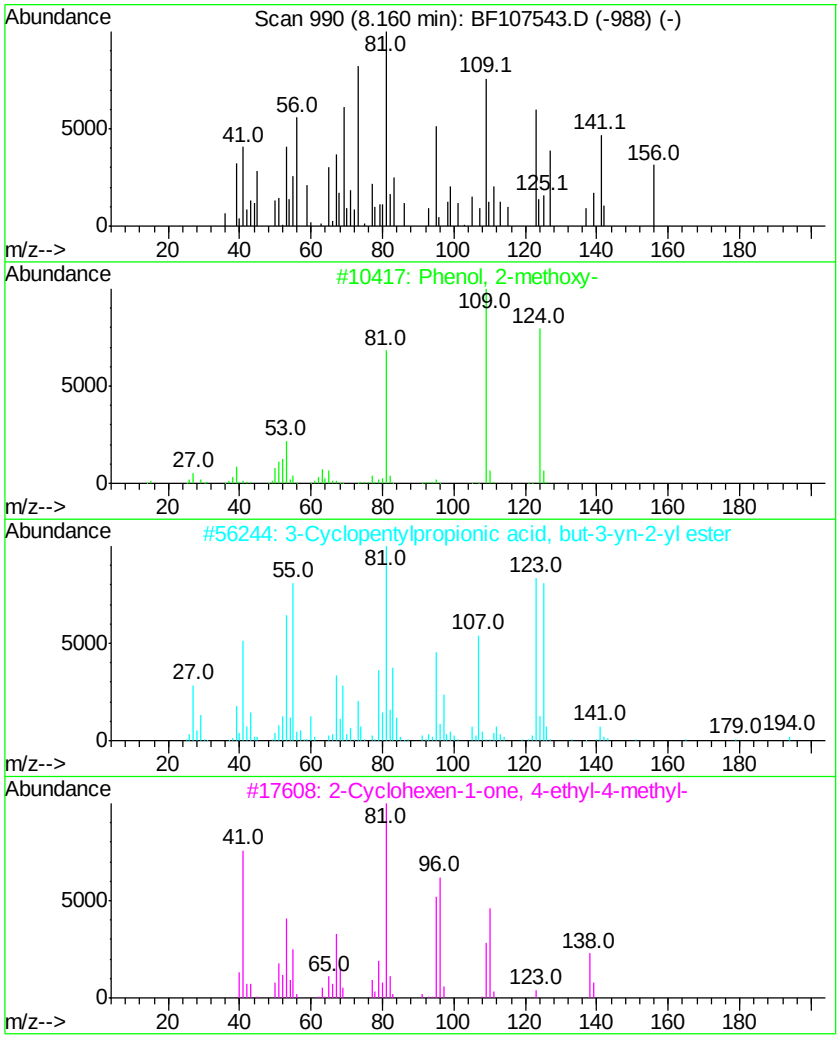
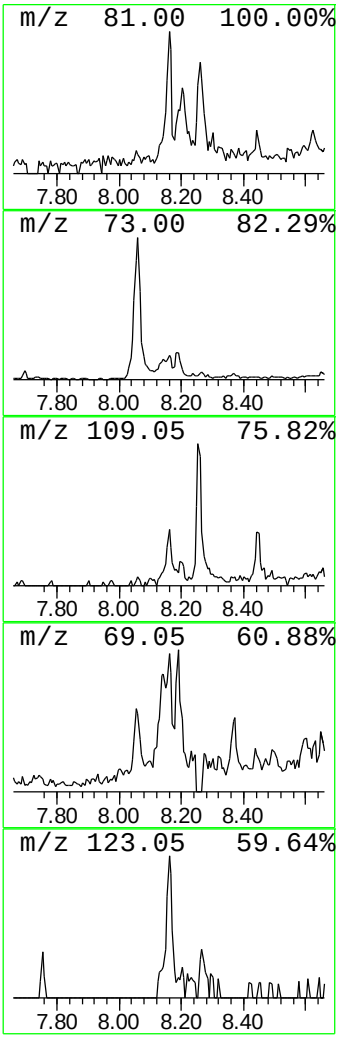
Peak Number 5 unknown8.16 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	2.37 ng	275645	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	47
2	3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	38
3	2-Cyclohexen-1-one, 4-ethyl-4-me...	138	C9H14O	017429-32-2	37
4	Pyridine, 3-methyl-, 1-oxide	109	C6H7NO	001003-73-2	35
5	Furan, 2-(methoxymethyl)-	112	C6H8O2	013679-46-4	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107543.D
Acq On : 21 Jul 2018 00:03
Operator : JU/SJ
Sample : J4018-02 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-3-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

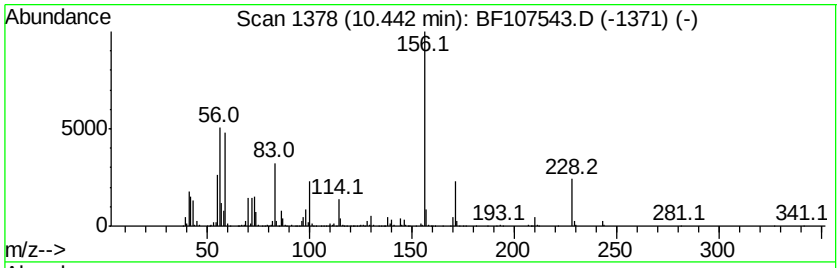
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

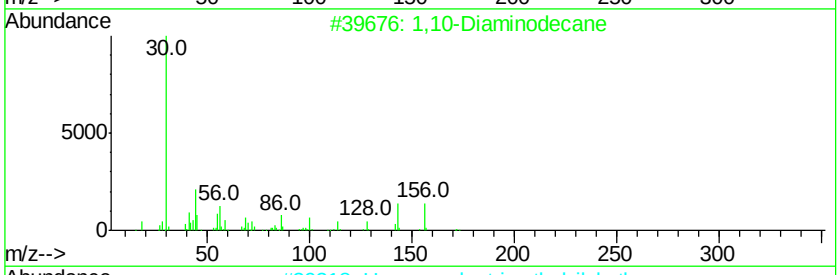
****

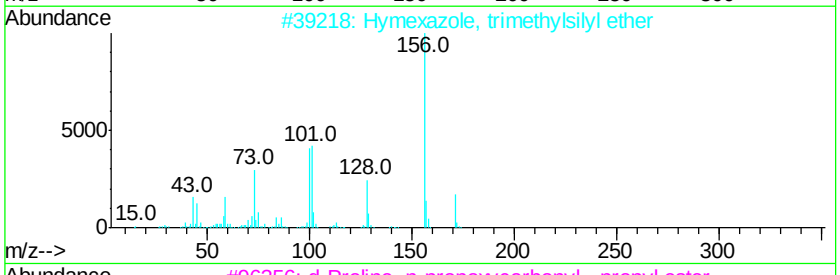
Peak Number 6 unknown10.44 Concentration Rank 1

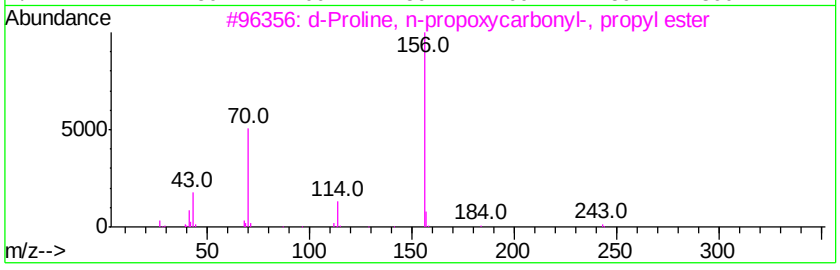
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	51.39 ng	6326850	Acenaphthene-d10	10.01

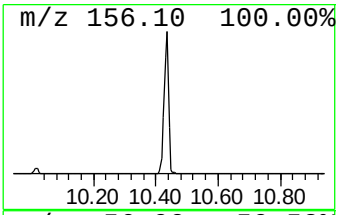
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,10-Diaminodecane	172	C10H24N2	000646-25-3	38
2	Hymexazole, trimethylsilyl ether	171	C7H13NO2Si	1000334-05-9	22
3	d-Proline, n-propoxycarbonyl-, p...	243	C12H21NO4	1000320-81-8	18
4	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	14
5	l-Proline, N-propoxycarbonyl-, p...	243	C12H21NO4	1000313-69-8	14

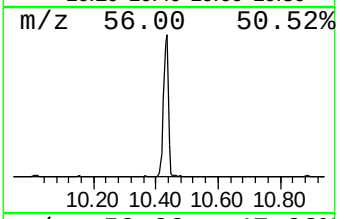


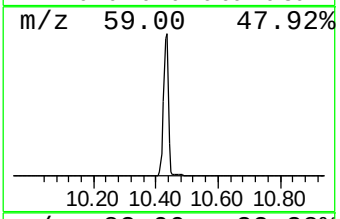


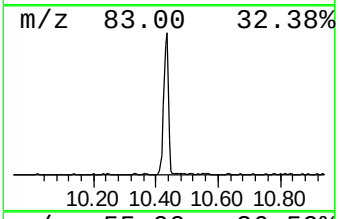


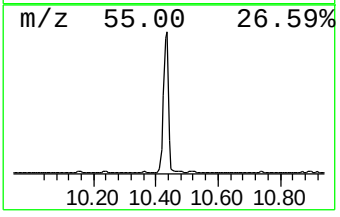












Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

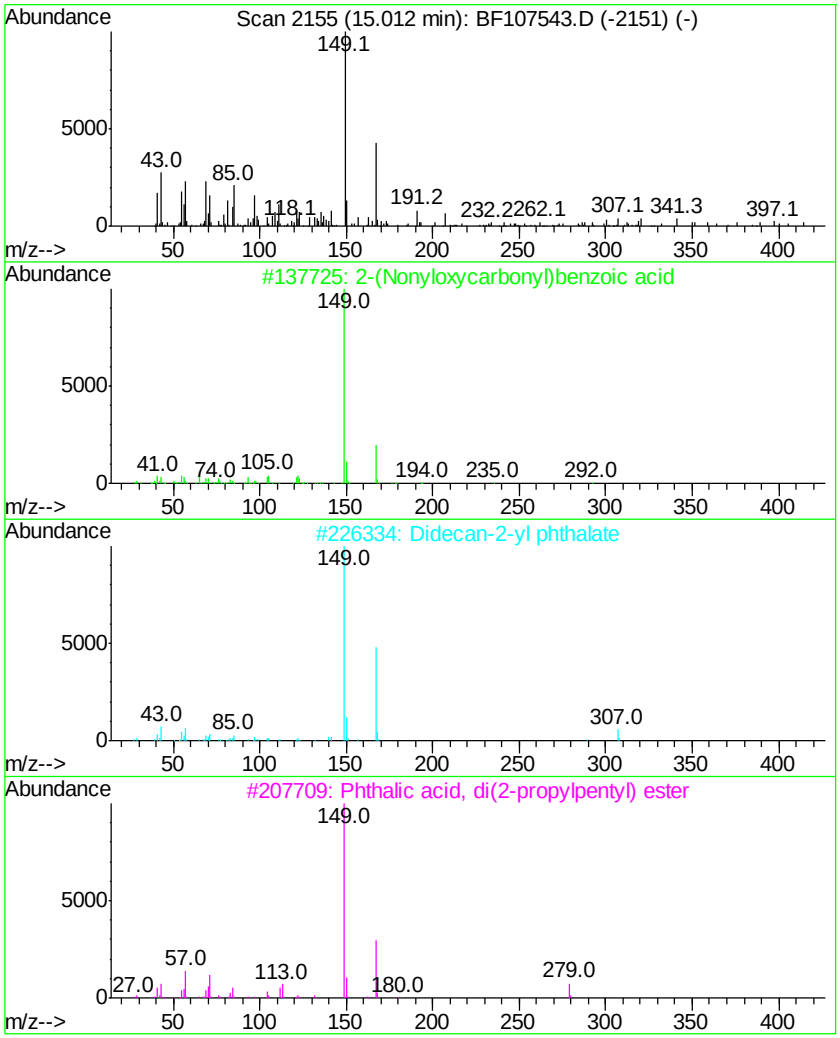
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

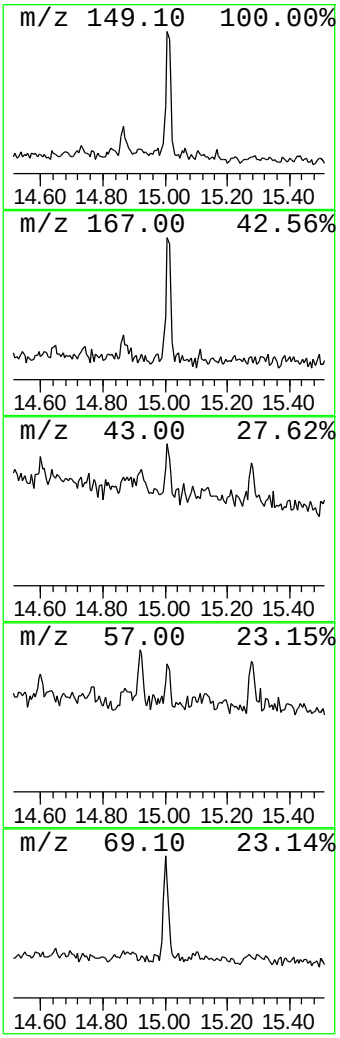
****

Peak Number 7 2-(Nonyloxycarbonyl)benzoic... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	2.26 ng	231839	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Nonyloxycarbonyl)benzoic acid	292	C17H24O4	1000373-89-9	55
2	Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	43
3	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	43
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	35
5	Phthalic acid, cyclohexylmethyl ...	332	C20H28O4	1000315-55-5	35





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.74	6.74	7.1	ng	646184	1	6.97	1816610	20.0
Valproic Acid	8.06	2.7	ng	314647	2	8.25	2323430	20.0
unknown8.14	8.14	3.2	ng	374360	2	8.25	2323430	20.0
unknown8.16	8.16	2.4	ng	275645	2	8.25	2323430	20.0
unknown10.44	10.44	51.4	ng	6326850	3	10.01	2462480	20.0
2-(Nonyloxycarbon...	15.01	2.3	ng	231839	6	15.69	2052290	20.0