LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108279.D
Acq On : 20 Aug 2018 10:25
Operator : JU/SJ
Sample : PB112152BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112152BL

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-BF080818.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	2.419	10	14	23	rVB	71502	109794	1.62%	0.220%
2	5.278	495	500	510	rBV	161040	219020	3.23%	0.438%
3	5.654	558	564	567	rBV	4702262	4798168	70.67%	9.596%
4	6.642	725	732	735	rBV	4725064	5010035	73.79%	10.020%
5	6.789	752	757	760	rBV	5109521	5005986	73.73%	10.012%
6	7.013	791	795	799	rBV	1315873	1167776	17.20%	2.336%
7	7.172	818	822	826	rBV	4250833	3956715	58.27%	7.913%
8	7.578	885	891	894	rBV	2974051	3368635	49.61%	6.737%
9	8.301	1009	1014	1017	rBV	1555649	1472404	21.69%	2.945%
10	9.378	1190	1197	1200	rBV	5725773	6220291	91.61%	12.440%
11	10.060	1308	1313	1325	rBV2	1853646	1778799	26.20%	3.558%
12	10.860	1443	1449	1452	rBV	4114545	4000721	58.92%	8.001%
13	11.560	1564	1568	1571	rBV	2275563	1887990	27.81%	3.776%
14	13.148	1833	1838	1841	rBV	6313268	6789773	100.00%	13.579%
15	13.477	1883	1894	1912	rVB3	68208	364615	5.37%	0.729%
16	14.071	1988	1995	2009	rBV	109930	479745	7.07%	0.959%
17	14.213	2015	2019	2023	rBV	1900610	1843857	27.16%	3.688%
18	15.777	2279	2285	2295	rVB	1052697	1526283	22.48%	3.053%

Sum of corrected areas: 50000607

LSC Report - Integrated Chromatogram

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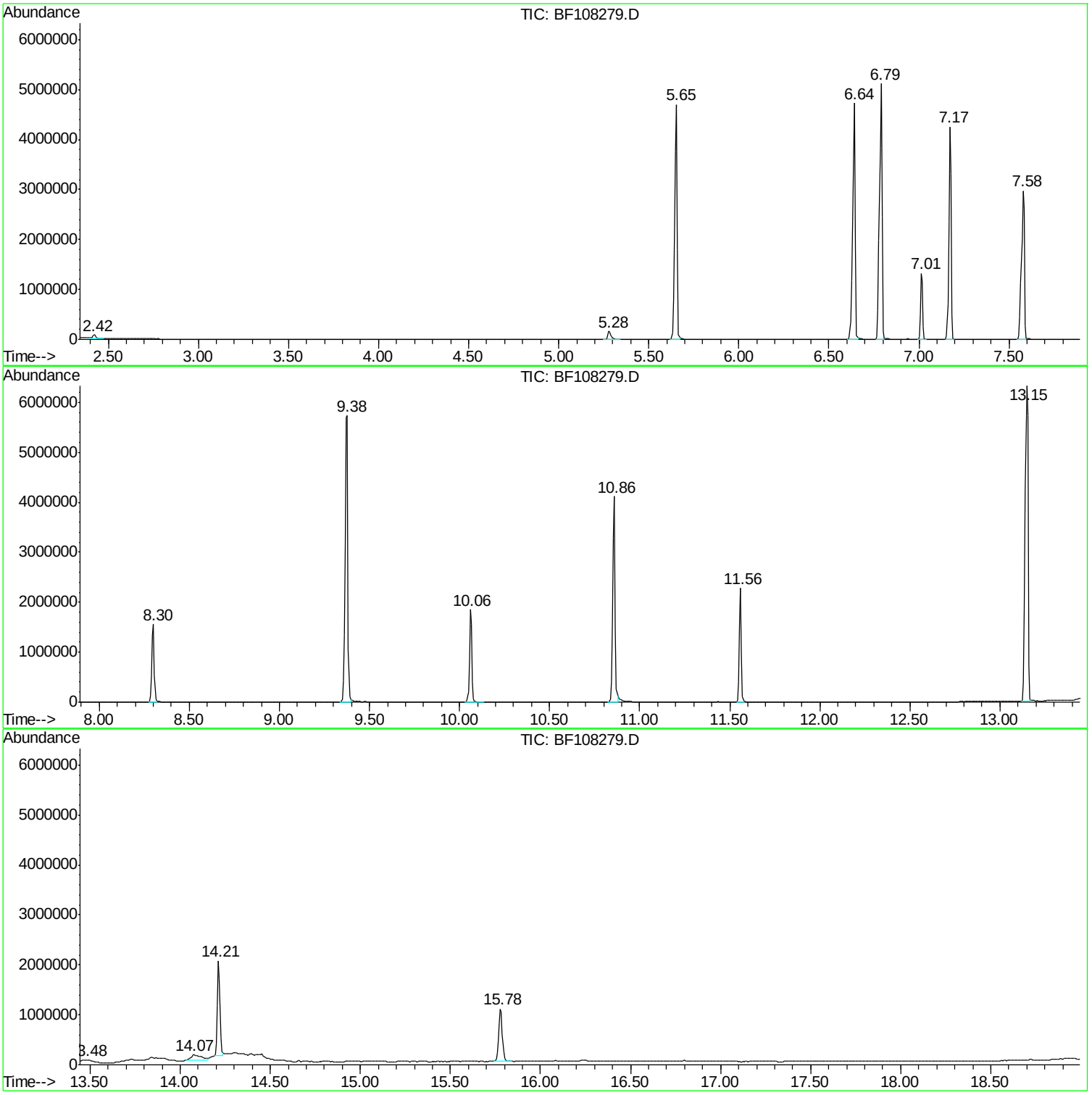
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB112152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF108279.D
Acq On : 20 Aug 2018 10:25
Operator : JU/SJ
Sample : PB112152BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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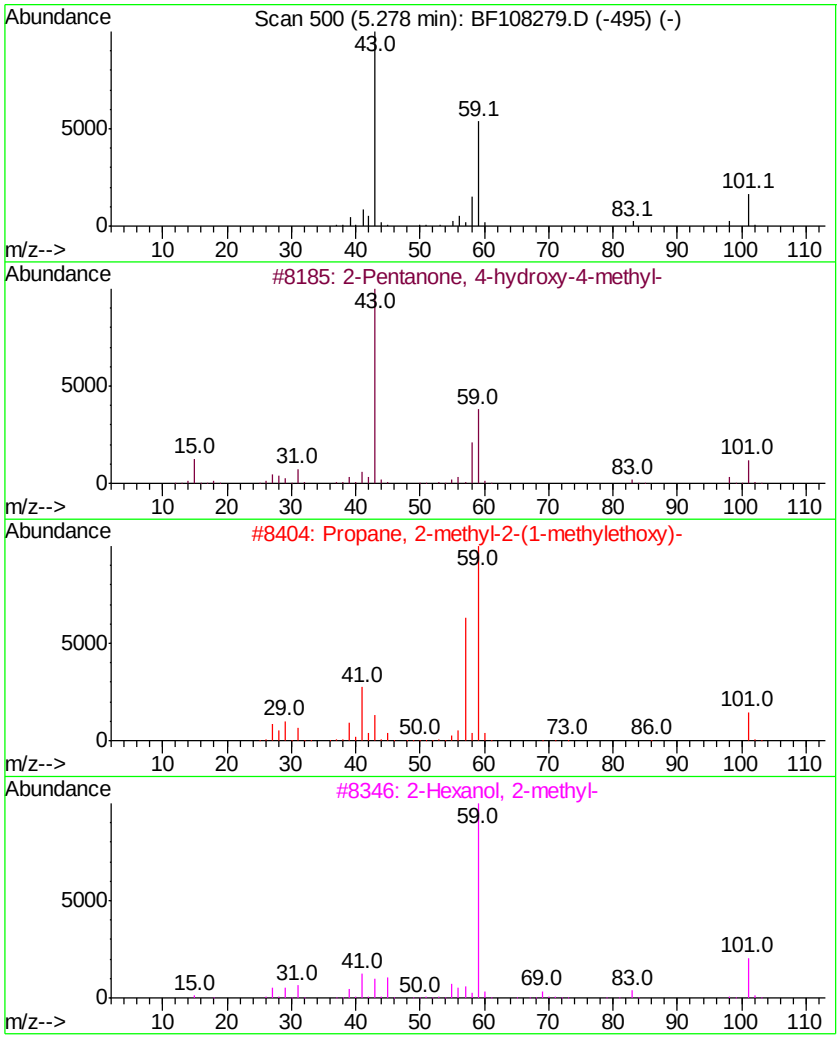
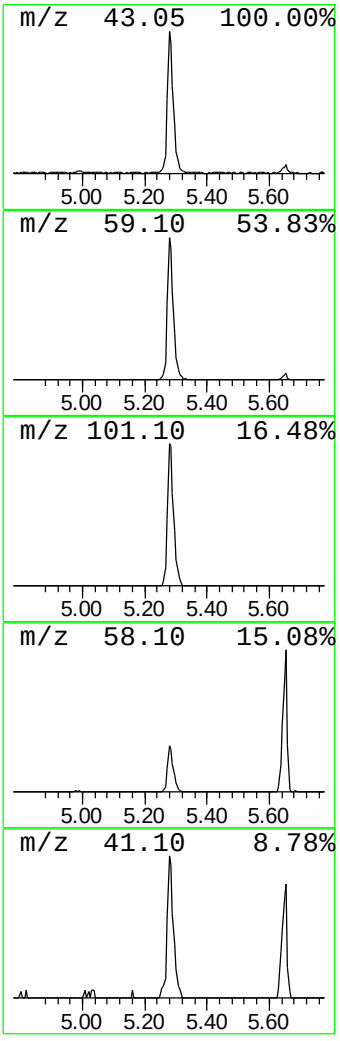
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.28	3.75 ng	219020	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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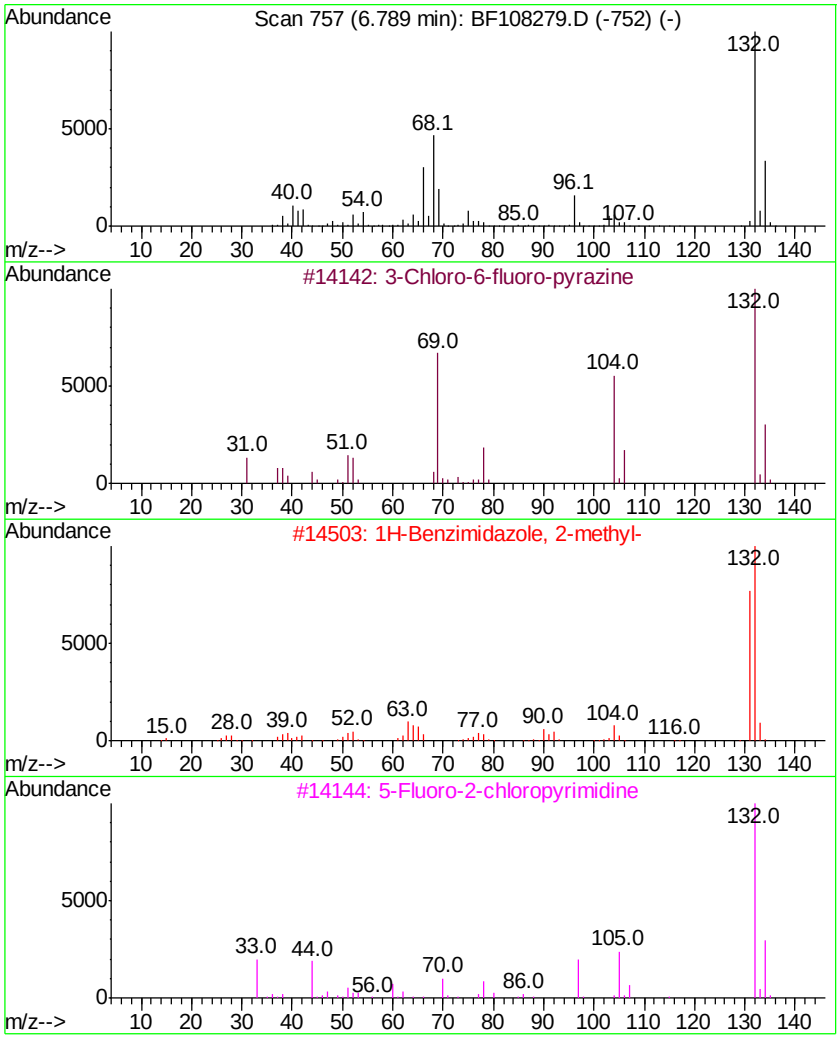
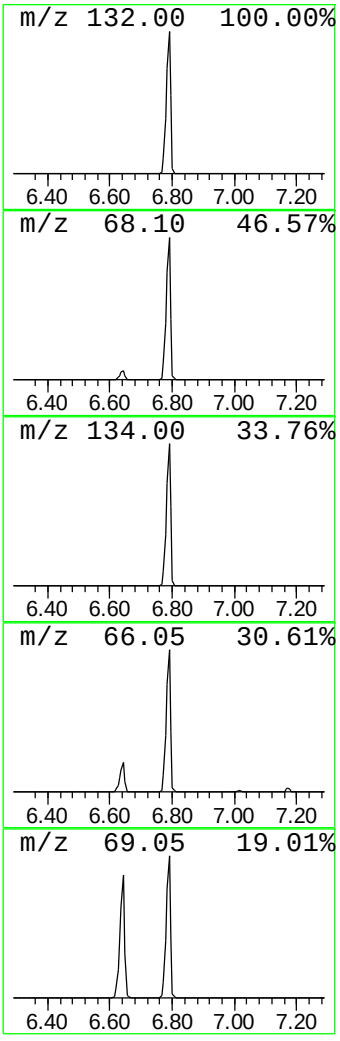
Peak Number 2 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	85.74 ng	5005990	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Sample : PB112152BL
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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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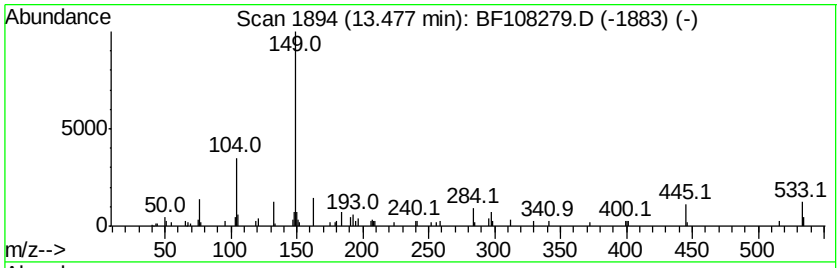
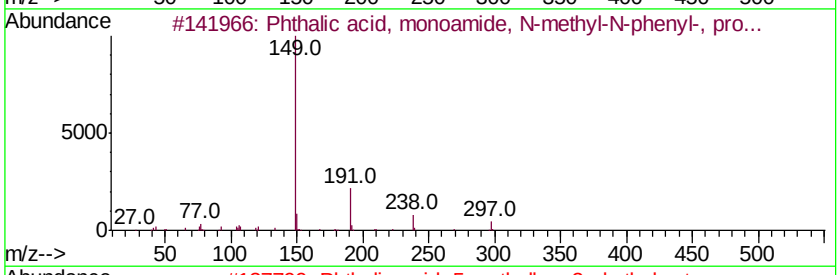
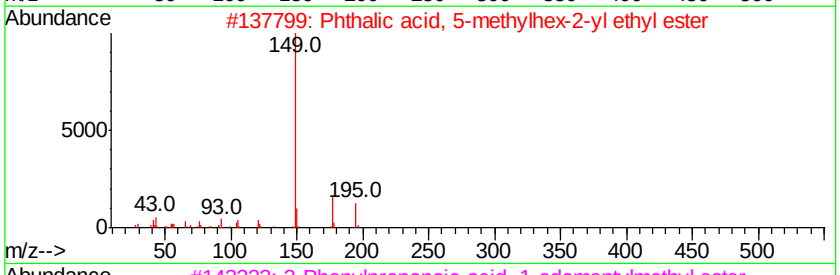
Peak Number 4 unknown13.48 Concentration Rank 4

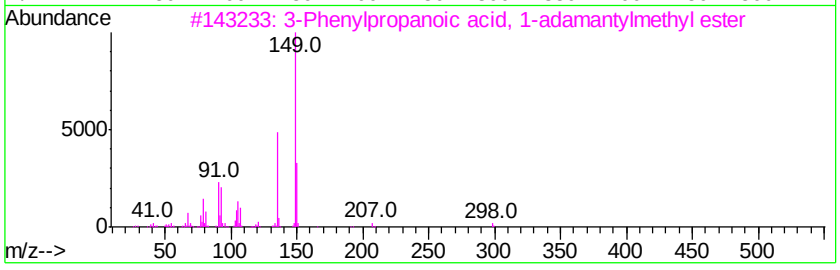
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	3.95 ng	364615	Chrysene-d12	14.21

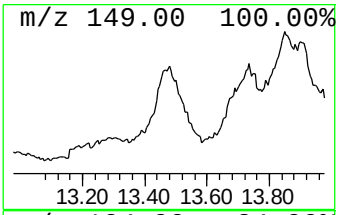
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, monoamide, N-meth...	297	C18H19NO3	1000322-83-9	47
2	Phthalic acid, 5-methylhex-2-yl ...	292	C17H24O4	1000371-09-3	43
3	3-Phenylpropanoic acid, 1-adaman...	298	C20H26O2	1000282-93-6	43
4	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	43
5	Dimethylmalonic acid, di(3-methy...	312	C19H20O4	1000363-61-8	43

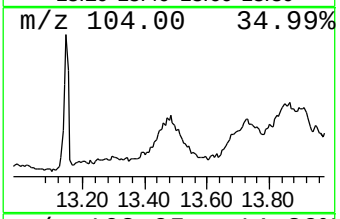


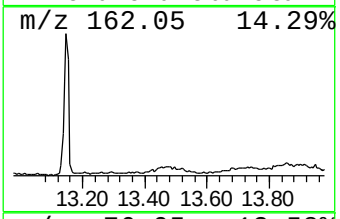


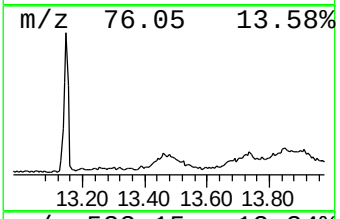


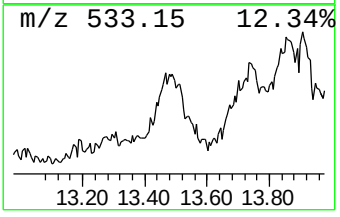












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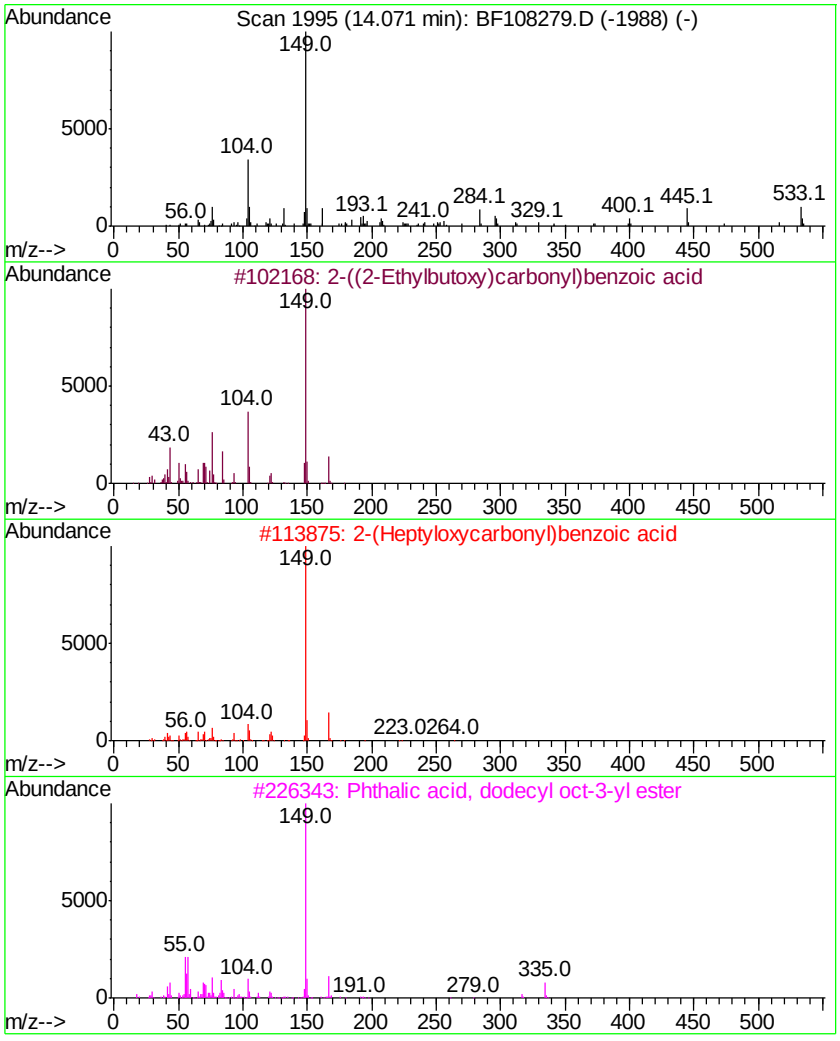
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

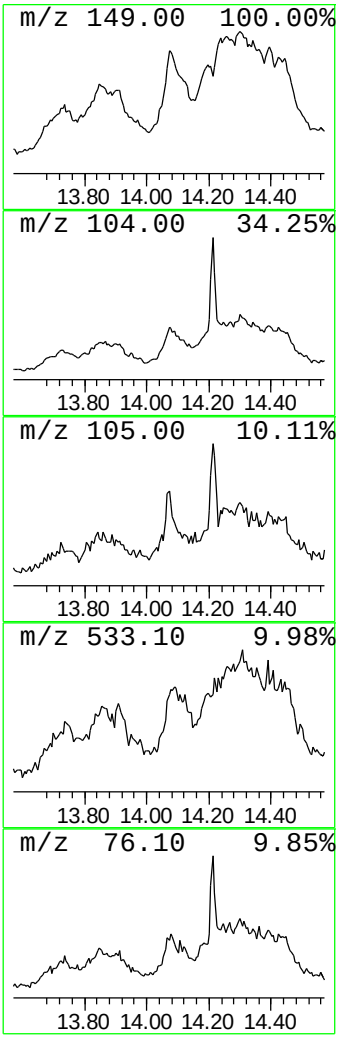
****

Peak Number 5 2-((2-Ethylbutoxy)carbonyl)... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	5.20 ng	479745	Chrysene-d12	14.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-((2-Ethylbutoxy)carbonyl)benzo...	250	C14H18O4	1000373-62-8	53
2	2-(Heptyloxycarbonyl)benzoic acid	264	C15H20O4	1000373-67-7	50
3	Phthalic acid, dodecyl oct-3-yl ...	446	C28H46O4	1000377-72-1	50
4	Phthalic acid, hexyl undec-2-en-...	402	C25H38O4	1000315-41-7	47
5	2-(Pentyloxycarbonyl)benzoic acid	236	C13H16O4	1000373-49-7	47





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.28	3.8	ng	219020	1	7.01	1167780	20.0
unknown6.79	6.79	85.7	ng	5005990	1	7.01	1167780	20.0
unknown13.48	13.48	4.0	ng	364615	5	14.21	1843860	20.0
2-((2-Ethylbutoxy...	14.07	5.2	ng	479745	5	14.21	1843860	20.0