LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087531.D
Acq On : 30 May 2016 2:15
Operator : UM/SJ
Sample : H3222-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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	3.781	190	192	200	rBV2	18090	92528	2.27%	0.344%
2	4.741	273	276	293	rBV	37298	196439	4.82%	0.730%
3	5.382	330	332	351	rBV	434271	1317699	32.35%	4.899%
4	7.039	475	477	482	rBV	305051	671705	16.49%	2.497%
5	7.119	482	484	502	rVB	1777957	3200085	78.56%	11.896%
6	7.473	513	515	527	rBV	464411	799873	19.64%	2.974%
7	7.702	532	535	552	rVB	1906445	2718668	66.74%	10.107%
8	8.388	592	595	607	rBV	1579439	2285761	56.11%	8.497%
9	9.508	690	693	716	rBV	516153	979846	24.05%	3.643%
10	11.279	845	848	866	rBV	3130156	4073495	100.00%	15.143%
11	12.011	908	912	923	rBV	27631	74699	1.83%	0.278%
12	12.331	938	940	956	rBV	688806	1086042	26.66%	4.037%
13	13.165	1009	1013	1015	rBV2	43240	74200	1.82%	0.276%
14	13.622	1050	1053	1078	rBV	1450255	2433251	59.73%	9.046%
15	13.931	1078	1080	1085	rBV	44621	76321	1.87%	0.284%
16	14.742	1149	1151	1168	rVB	496809	1010931	24.82%	3.758%
17	15.165	1184	1188	1196	rBV	27270	88038	2.16%	0.327%
18	16.834	1331	1334	1340	rBV	56549	153579	3.77%	0.571%
19	16.926	1340	1342	1345	rVB	268497	291682	7.16%	1.084%
20	17.040	1350	1352	1354	rVV	36477	40880	1.00%	0.152%
21	17.086	1354	1356	1370	rVV	2921796	3505680	86.06%	13.033%
22	17.851	1421	1423	1426	rBV2	157122	184041	4.52%	0.684%
23	18.171	1448	1451	1459	rVB2	22762	64750	1.59%	0.241%
24	18.457	1474	1476	1491	rBV	344591	707173	17.36%	2.629%
25	20.137	1622	1623	1638	rBV3	192885	606693	14.89%	2.255%
26	22.332	1812	1815	1817	rVB2	52512	58420	1.43%	0.217%
27	22.606	1837	1839	1842	rVB	30546	48855	1.20%	0.182%
28	23.429	1908	1911	1913	rVB4	49875	58142	1.43%	0.216%

Sum of corrected areas: 26899476

LSC Report - Integrated Chromatogram

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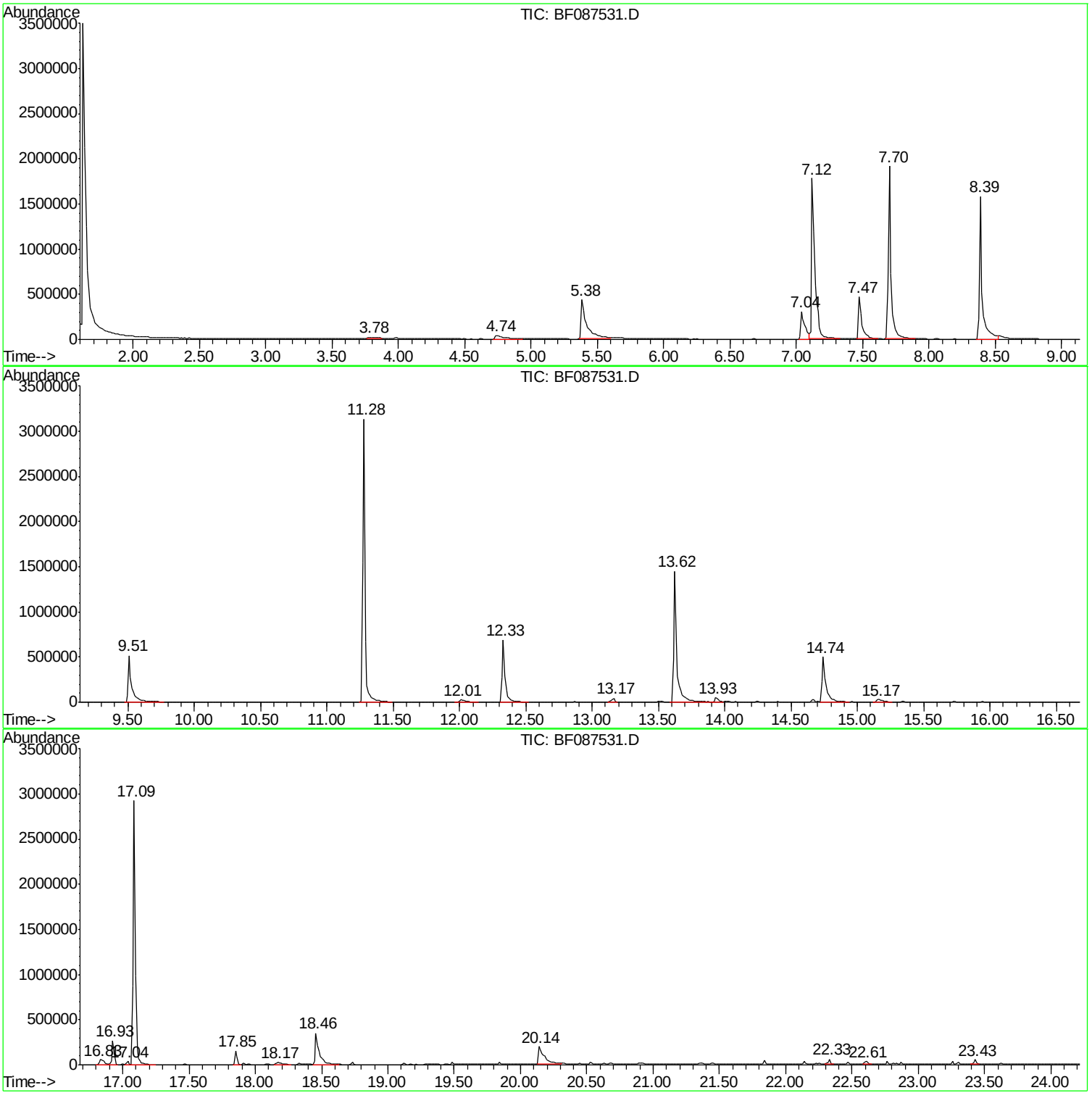
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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 : BF087531.D
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Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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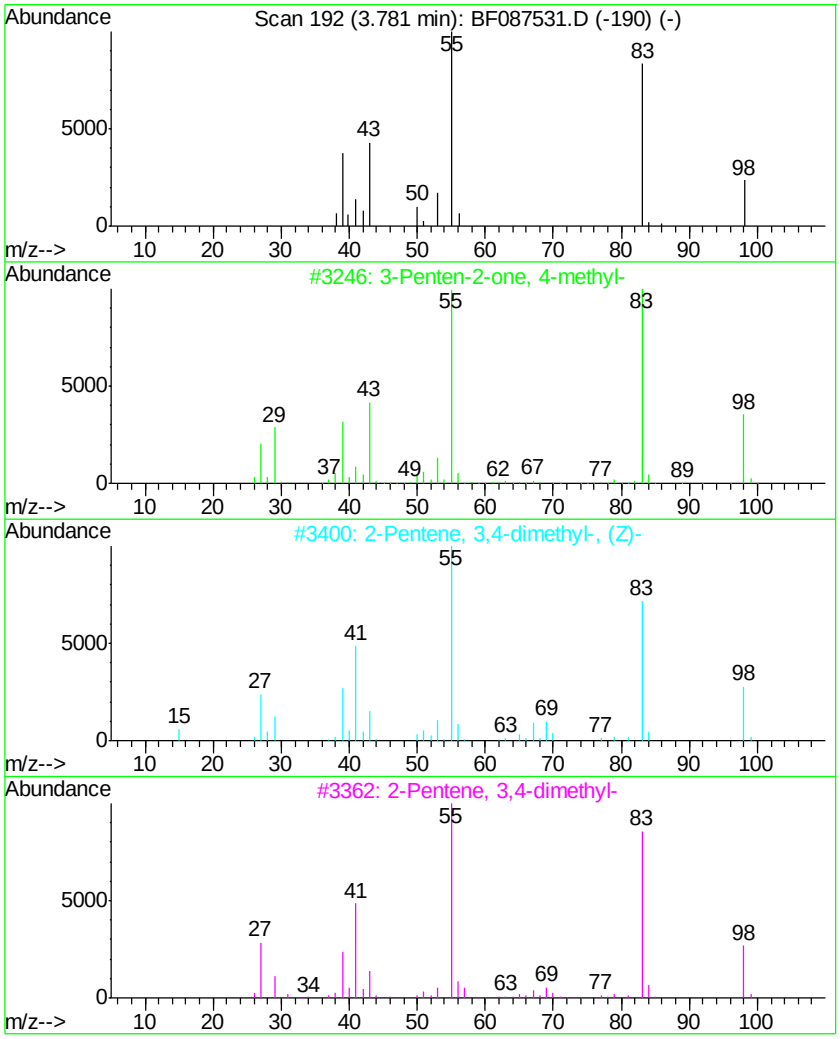
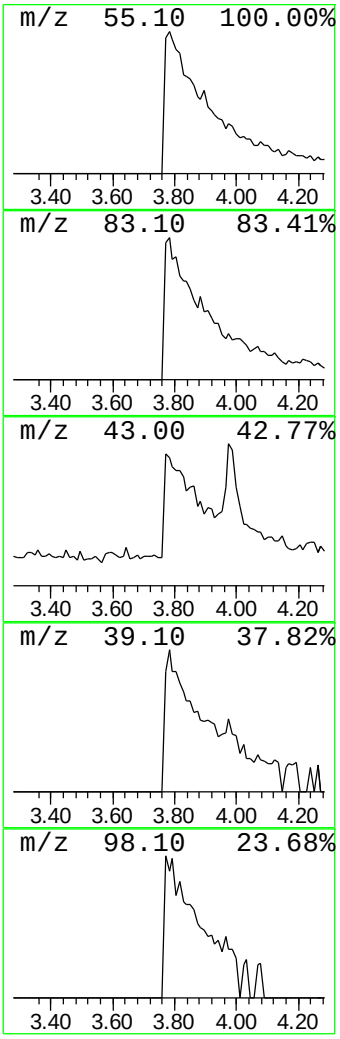
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.78	2.31 ng	92528	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	78
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	45
5	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	45





Library Search Compound Report

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Data File : BF087531.D
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Operator : UM/SJ
Sample : H3222-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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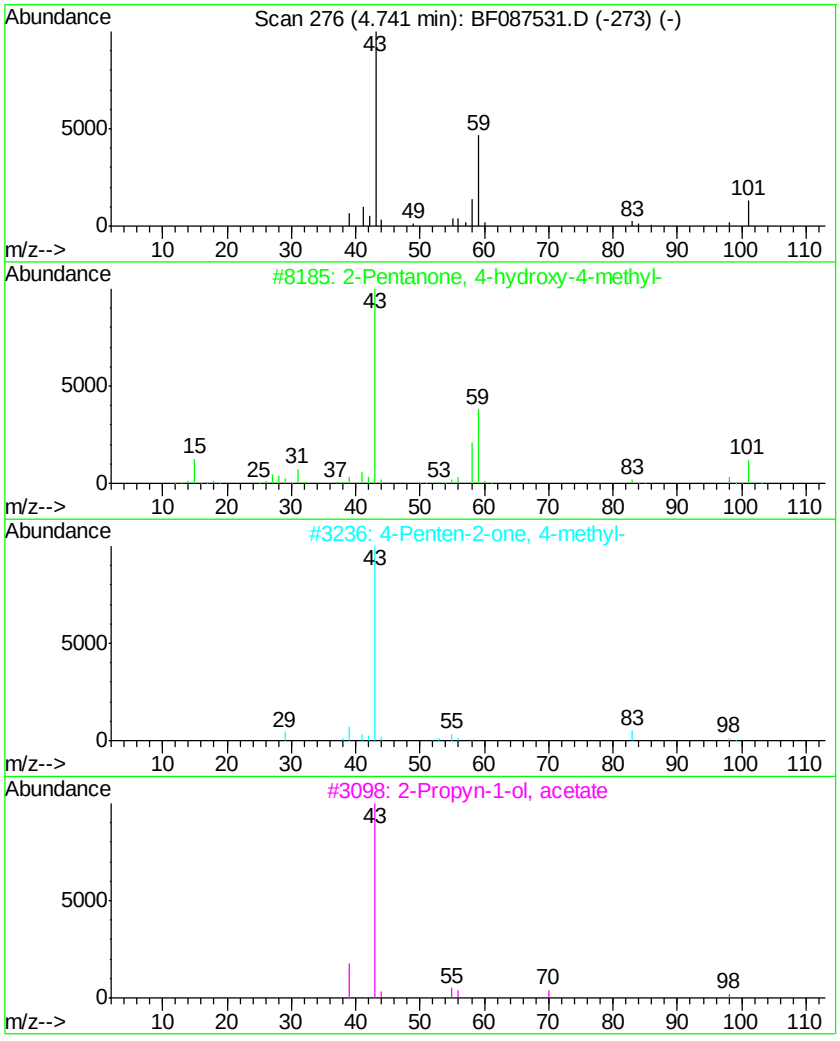
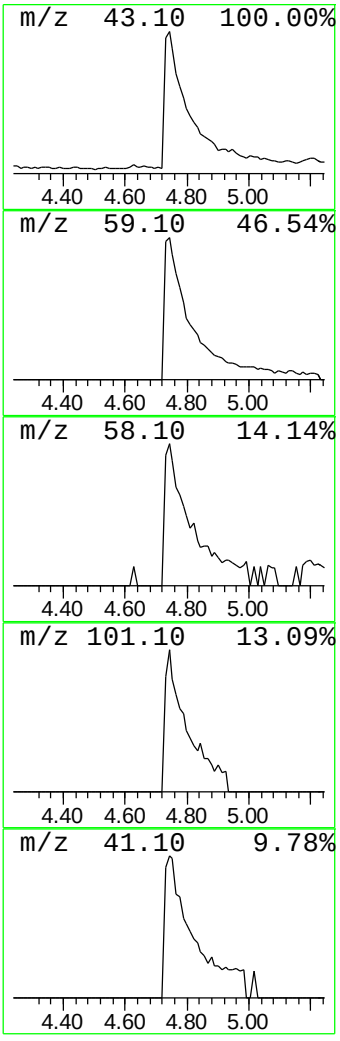
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	4.91 ng	196439	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087531.D
Acq On : 30 May 2016 2:15
Operator : UM/SJ
Sample : H3222-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

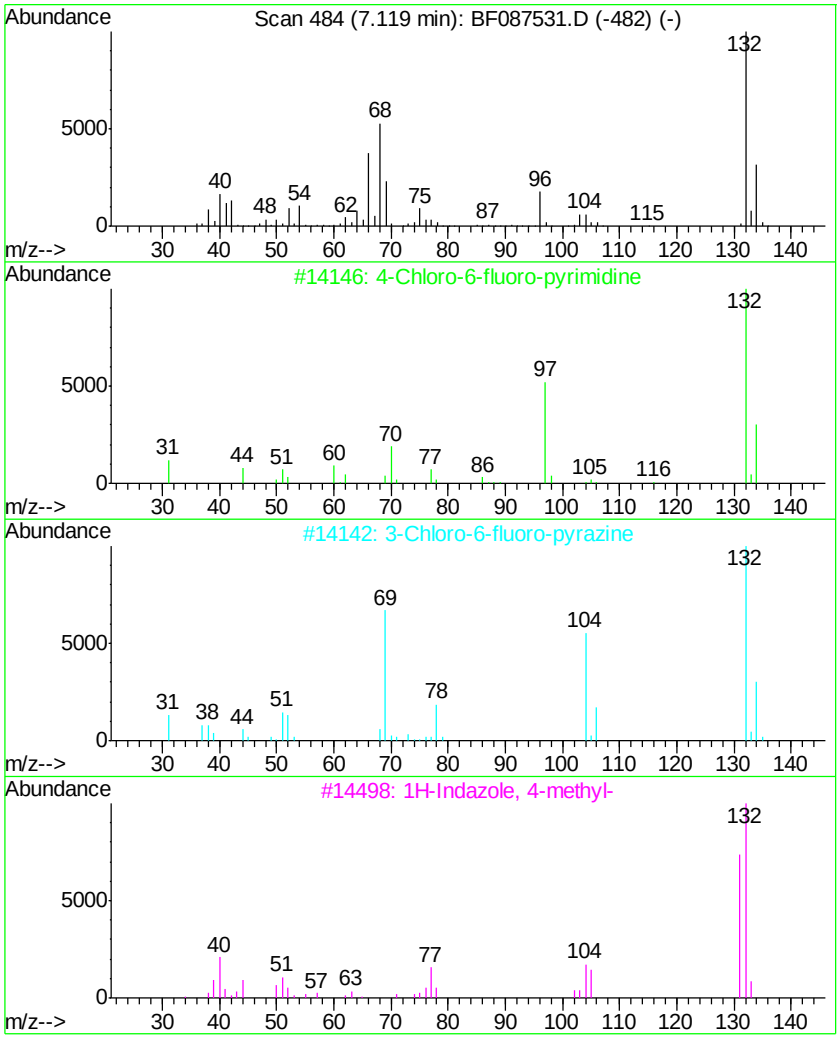
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

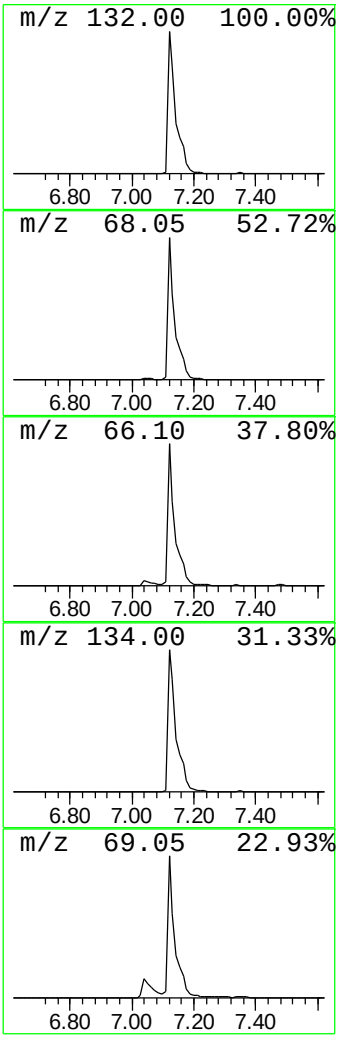
****

Peak Number 3 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	80.01 ng	3200090	1,4-Dichlorobenzene-d4	7.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Indazole, 4-methyl-	132	C8H8N2	1000316-00-9	25
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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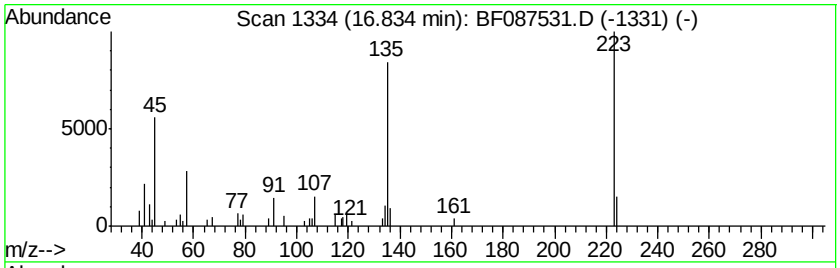
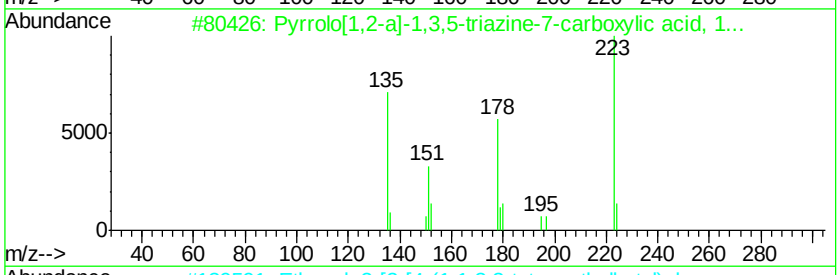
****

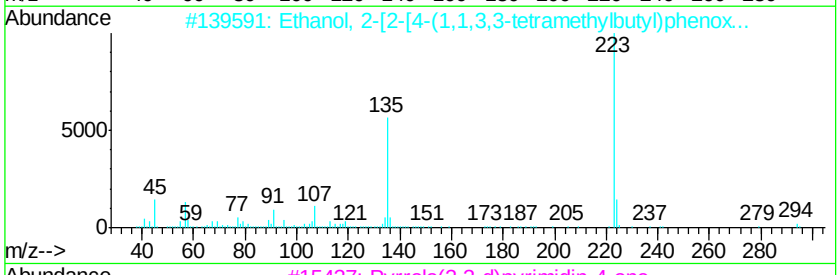
Peak Number 5 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 6

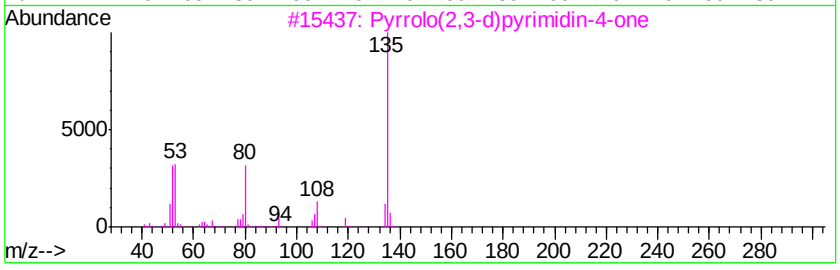
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	4.34 ng	153579	Chrysene-d12	18.46

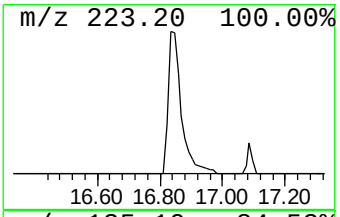
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	58
3	Pyrrolo(2,3-d)pyrimidin-4-one	135	C6H5N3O	003680-71-5	30
4	2-Hydroxy-5-methylbenzohydrazide	166	C8H10N2O2	028397-43-5	27
5	3,5-Dihydropyrrolo(3,2-d)pyrimid...	135	C6H5N3O	005655-01-6	27

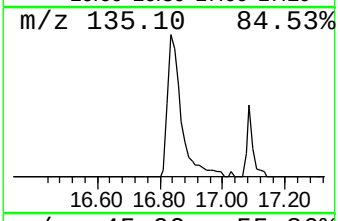


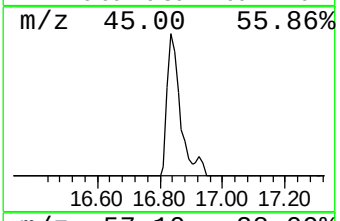


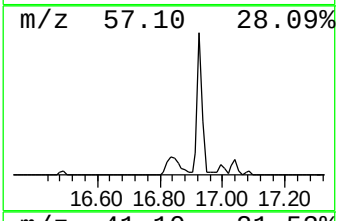


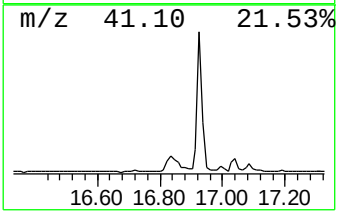












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

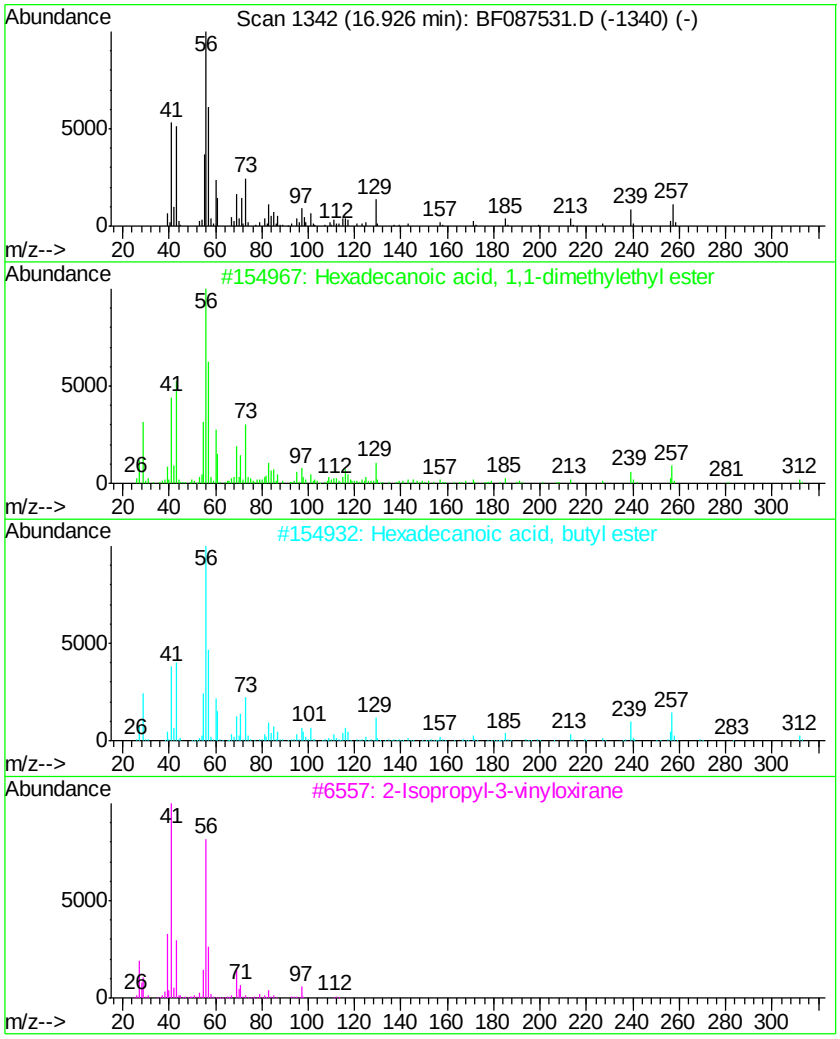
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

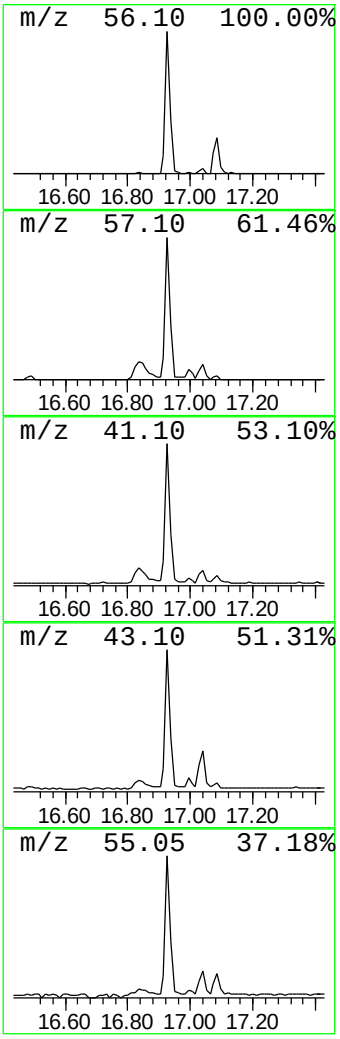
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	8.25 ng	291682	Chrysene-d12	18.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
3	2-Isopropyl-3-vinyloxirane	112	C7H12O	070777-23-0	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38





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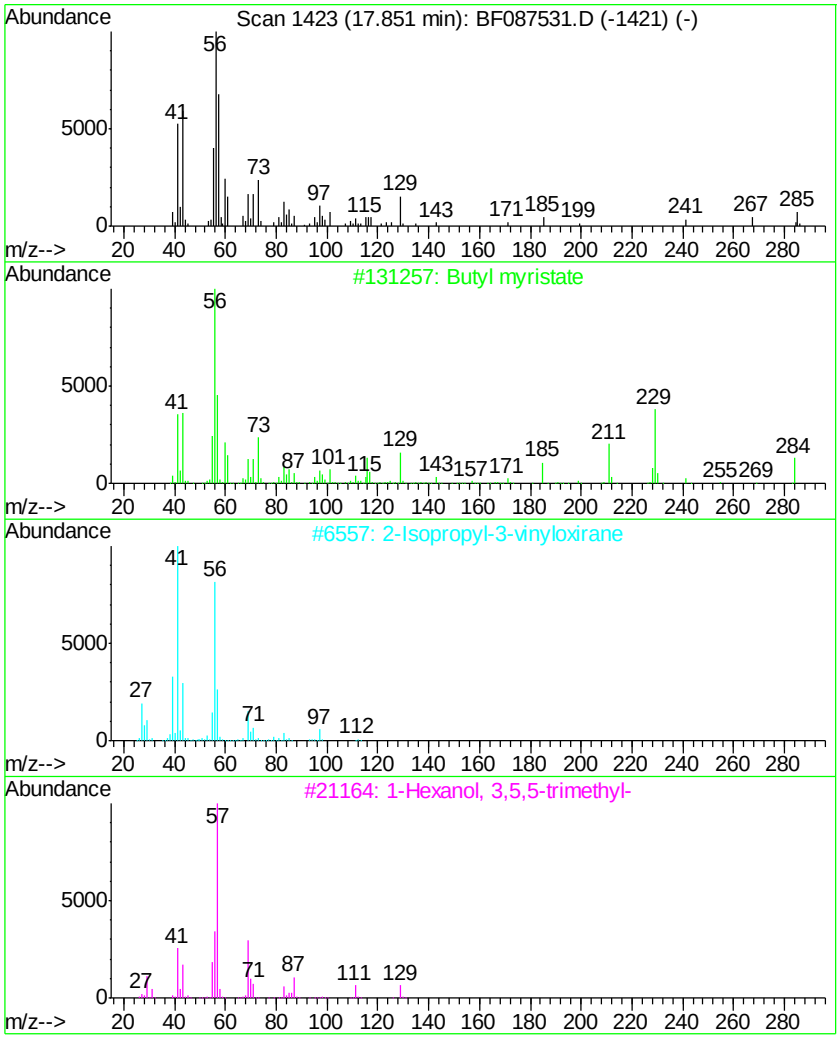
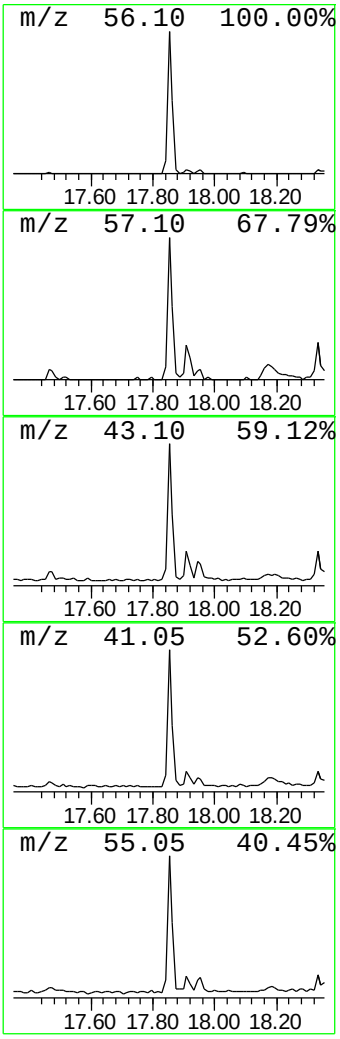
****

Peak Number 7 Butyl myristate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	5.20 ng	184041	Chrysene-d12	18.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	86
2	2-Isopropyl-3-vinyloxirane	112	C7H12O	070777-23-0	43
3	1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38





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
3-Penten-2-one, 4...	3.78	2.3	ng	92528	1	7.47	799873	20.0
2-Pentanone, 4-hy...	4.74	4.9	ng	196439	1	7.47	799873	20.0
unknown7.12	7.12	80.0	ng	3200090	1	7.47	799873	20.0
Pyrrolo[1,2-a]-1,...	16.83	4.3	ng	153579	5	18.46	707173	20.0
Hexadecanoic acid...	16.93	8.3	ng	291682	5	18.46	707173	20.0
Butyl myristate	17.85	5.2	ng	184041	5	18.46	707173	20.0