LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087895.D
Acq On : 11 Jun 2016 1:58
Operator : UM/SJ
Sample : H3440-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-17

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-BF060716.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	1.747	12	14	23	rVB	261273	511263	9.13%	1.952%
2	1.873	23	25	92	rVB	2447179	5601094	100.00%	21.382%
3	4.970	294	296	300	rBV	58497	74335	1.33%	0.284%
4	5.404	331	334	336	rVB	1311105	1285106	22.94%	4.906%
5	6.444	422	425	427	rBV	911492	870360	15.54%	3.323%
6	6.582	434	437	439	rBV	2061226	2207216	39.41%	8.426%
7	6.810	455	457	459	rBV	703272	581703	10.39%	2.221%
8	6.970	468	471	473	rBV	2219784	2025314	36.16%	7.732%
9	7.153	484	487	489	rBV2	65985	114946	2.05%	0.439%
10	7.382	502	507	509	rBV	1763236	2182286	38.96%	8.331%
11	7.462	512	514	516	rBV	70608	60290	1.08%	0.230%
12	7.507	516	518	520	rBV	73500	60646	1.08%	0.232%
13	7.587	521	525	527	rVB	178134	171382	3.06%	0.654%
14	7.747	537	539	541	rBV2	56154	93071	1.66%	0.355%
15	7.793	541	543	544	rVB2	45908	56766	1.01%	0.217%
16	7.839	544	547	549	rBV	509975	459234	8.20%	1.753%
17	8.102	567	570	571	rVV	787578	821456	14.67%	3.136%
18	8.147	571	574	576	rVB2	133956	188978	3.37%	0.721%
19	8.479	602	603	607	rVB	64023	64417	1.15%	0.246%
20	8.570	607	611	612	rBV2	46832	68929	1.23%	0.263%
21	8.948	641	644	646	rVB2	31064	61358	1.10%	0.234%
22	9.016	646	650	651	rBV2	29231	75341	1.35%	0.288%
23	9.176	661	664	666	rVB	3089521	2721234	48.58%	10.388%
24	9.850	720	723	725	rBV	693280	705334	12.59%	2.693%
25	10.628	789	791	794	rBV2	887545	1214532	21.68%	4.636%
26	11.325	850	852	854	rVB	775927	613973	10.96%	2.344%
27	12.914	988	991	993	rBV	2011102	2315774	41.35%	8.840%
28	13.954	1079	1082	1084	rBV	520887	574098	10.25%	2.192%
29	15.360	1202	1205	1208	rBV	354763	415088	7.41%	1.585%

Sum of corrected areas: 26195524

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ClientSampleId :
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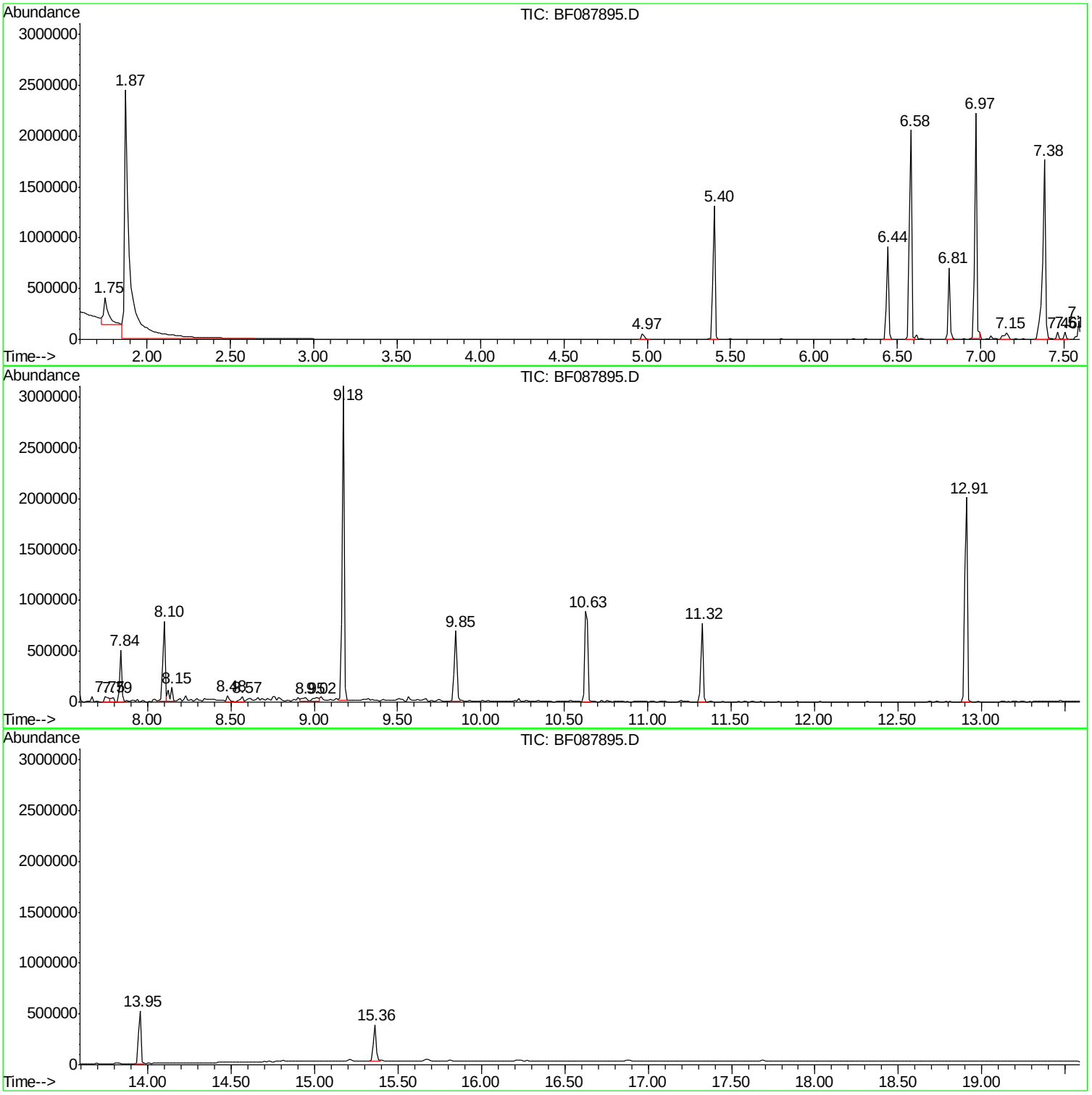
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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

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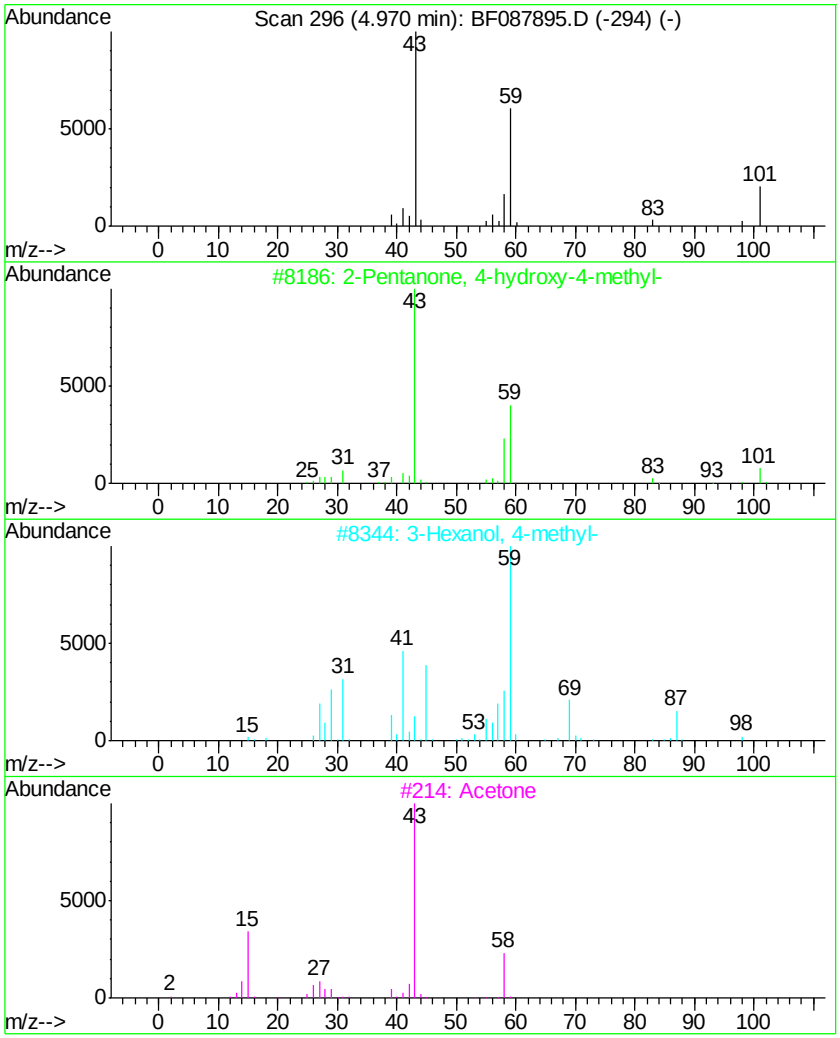
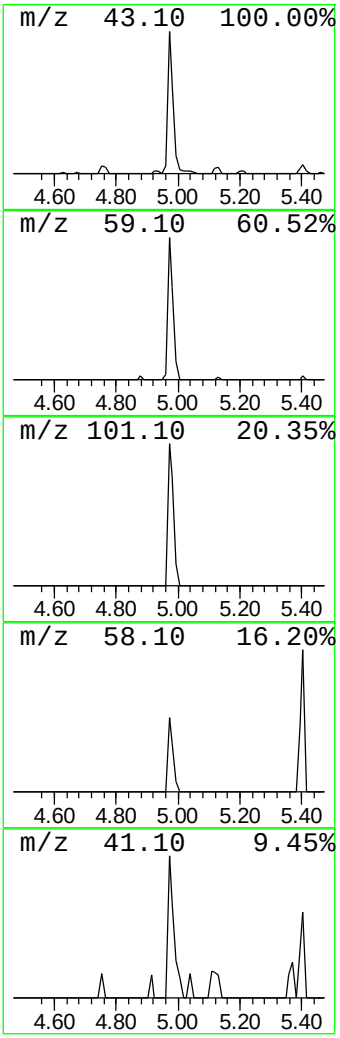
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.56 ng	74335	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetone	58	C3H6O	000067-64-1	9
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9





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Operator : UM/SJ
Sample : H3440-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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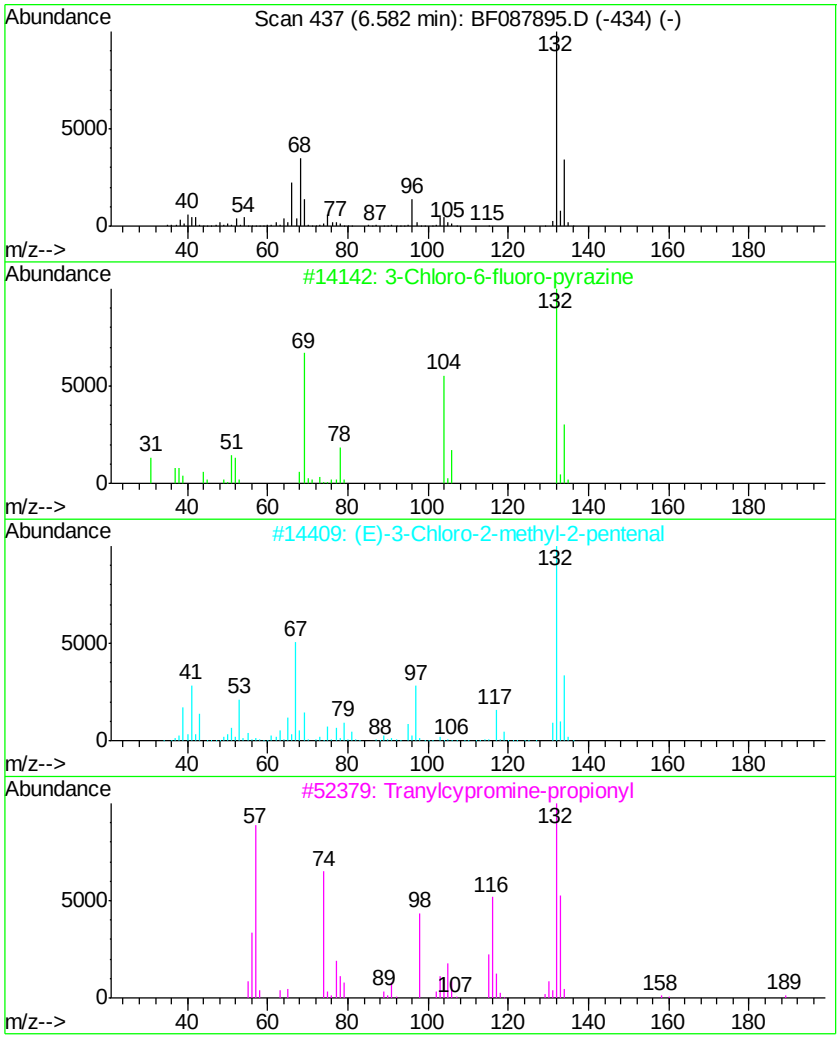
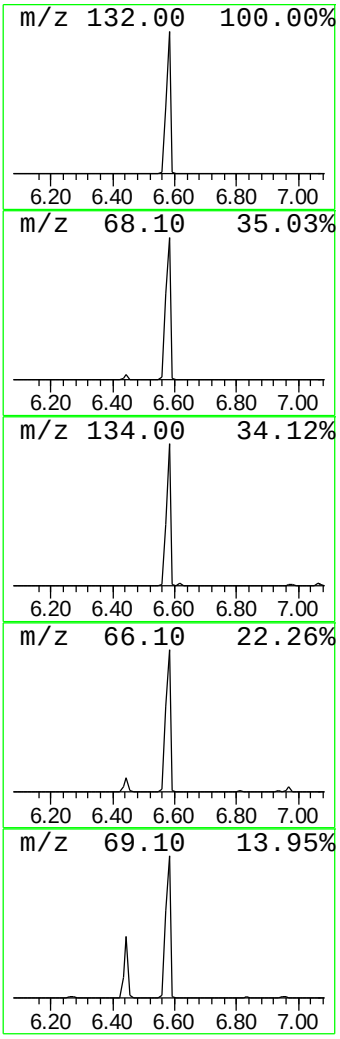
Peak Number 4 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	75.89 ng	2207220	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087895.D
Acq On : 11 Jun 2016 1:58
Operator : UM/SJ
Sample : H3440-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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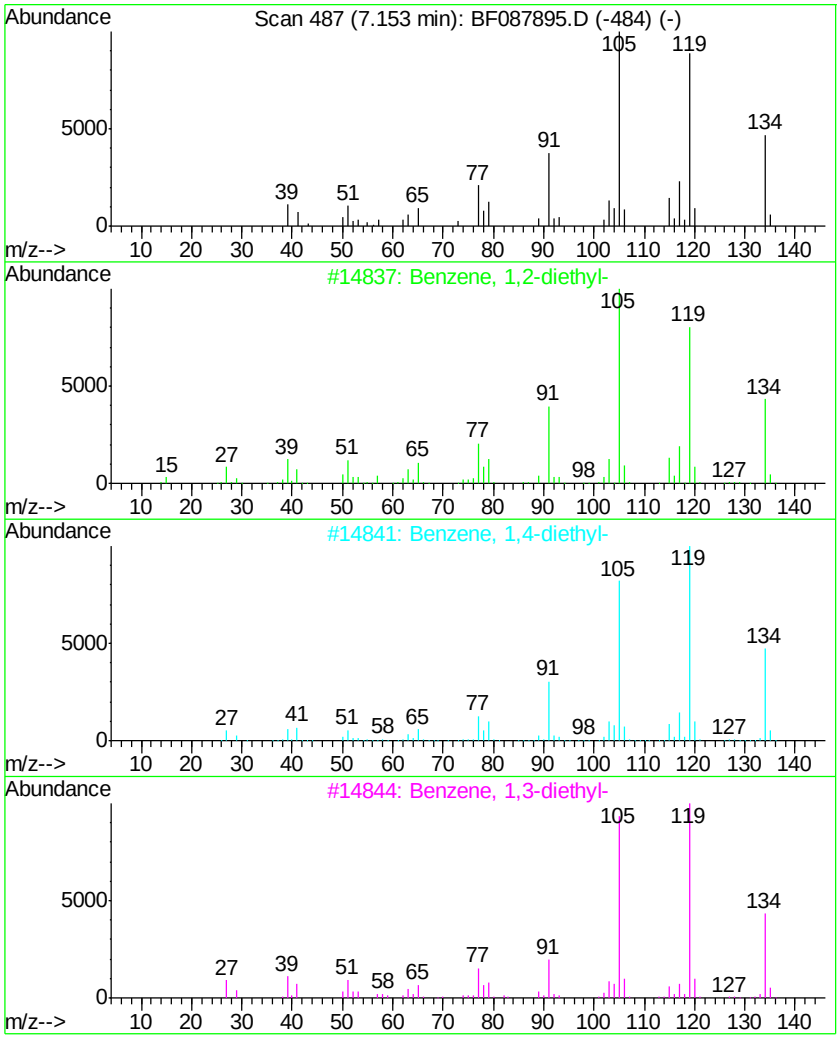
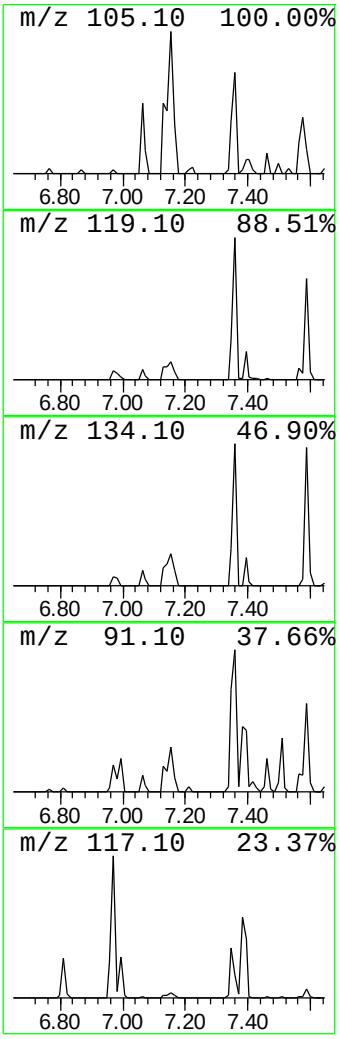
Peak Number 6 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	3.95 ng	114946	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	98
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	90
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76
5	o-Cymene	134	C10H14	000527-84-4	74





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Instrument : BNA_F
ClientSampleId : W-17

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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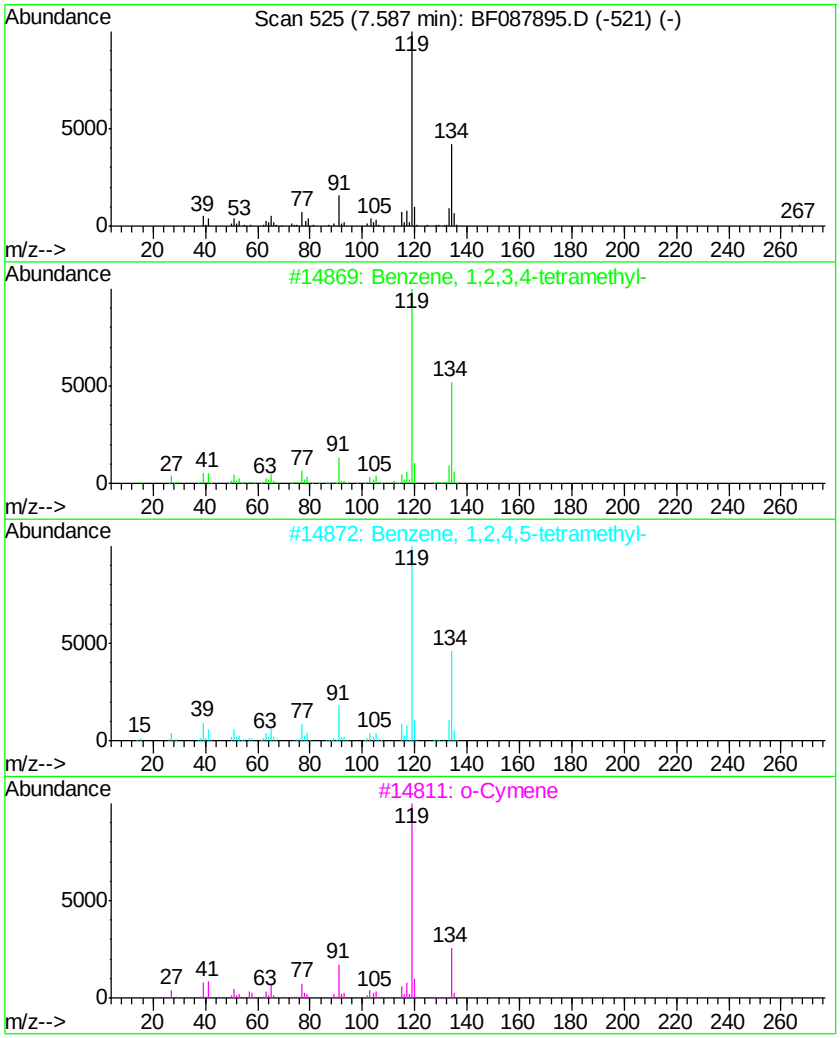
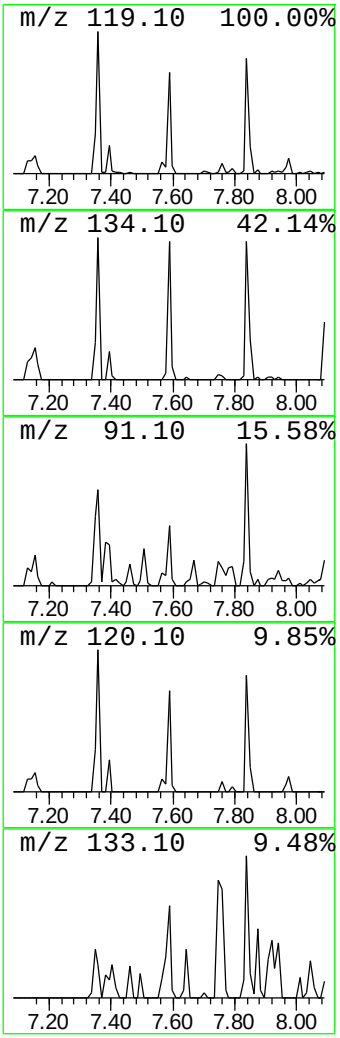
Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	4.17 ng	171382	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	o-Cymene	134	C10H14	000527-84-4	96
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93





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Sample : H3440-02
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ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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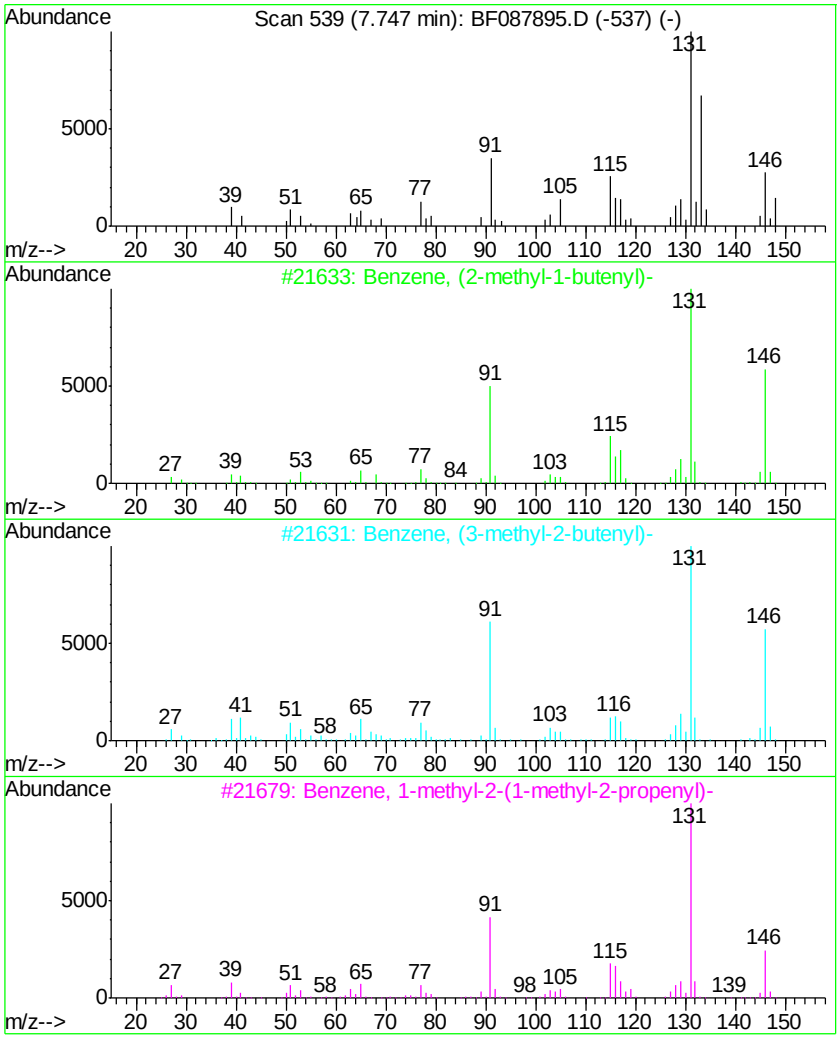
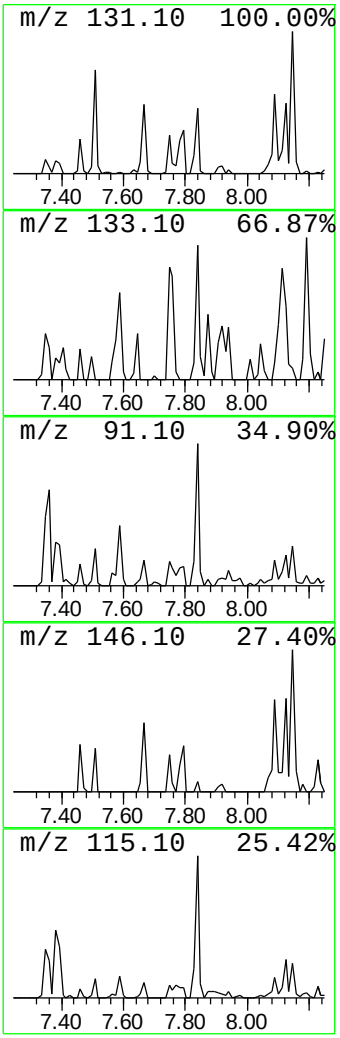
Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	2.27 ng	93071	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	95
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	94
3	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	93
4	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	92
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	89





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Instrument : BNA_F
ClientSampleId : W-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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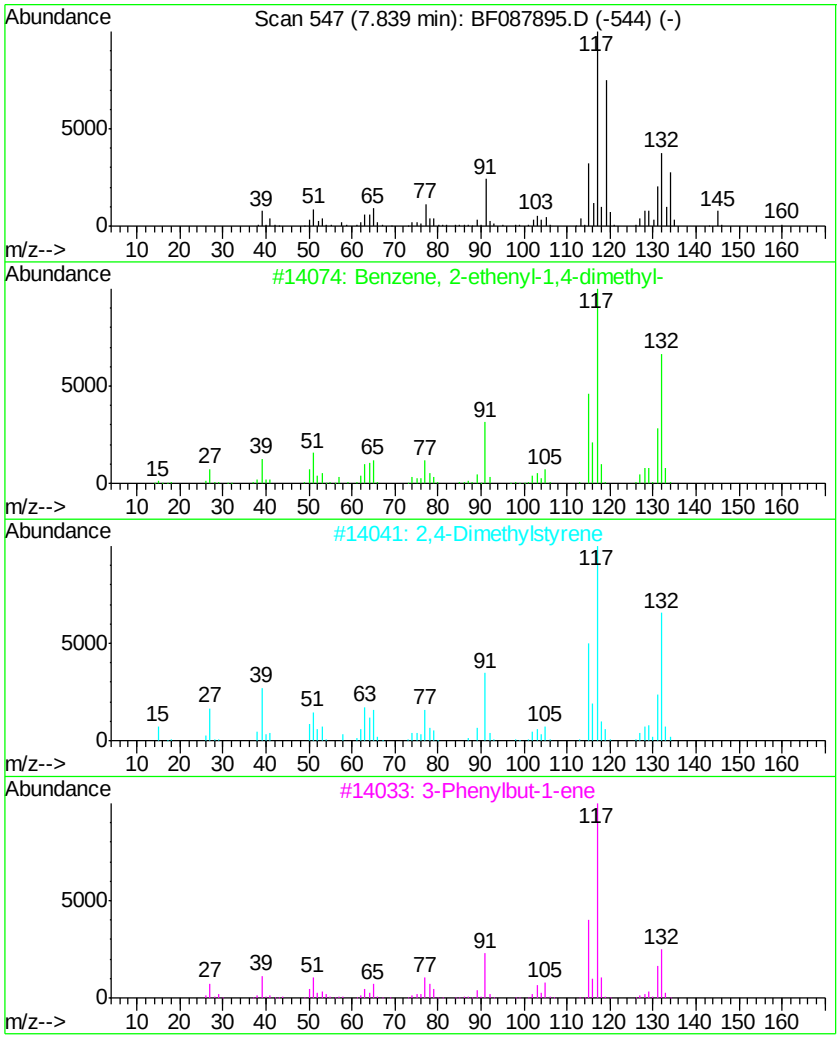
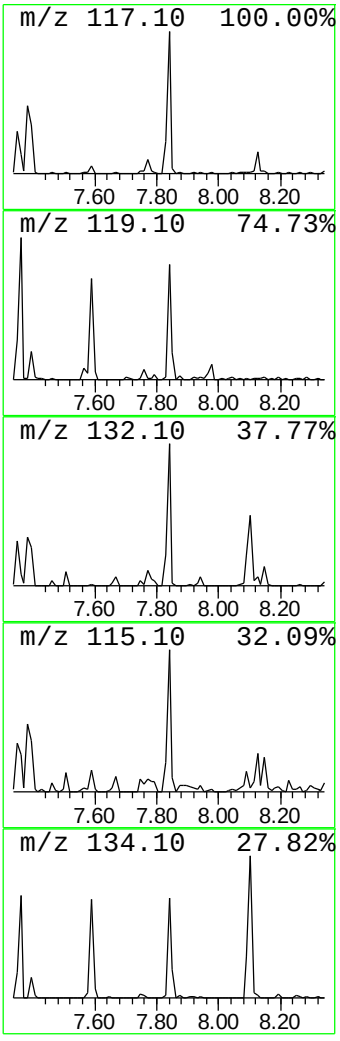
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	11.18 ng	459234	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	89
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	80
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	60
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	60
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	55





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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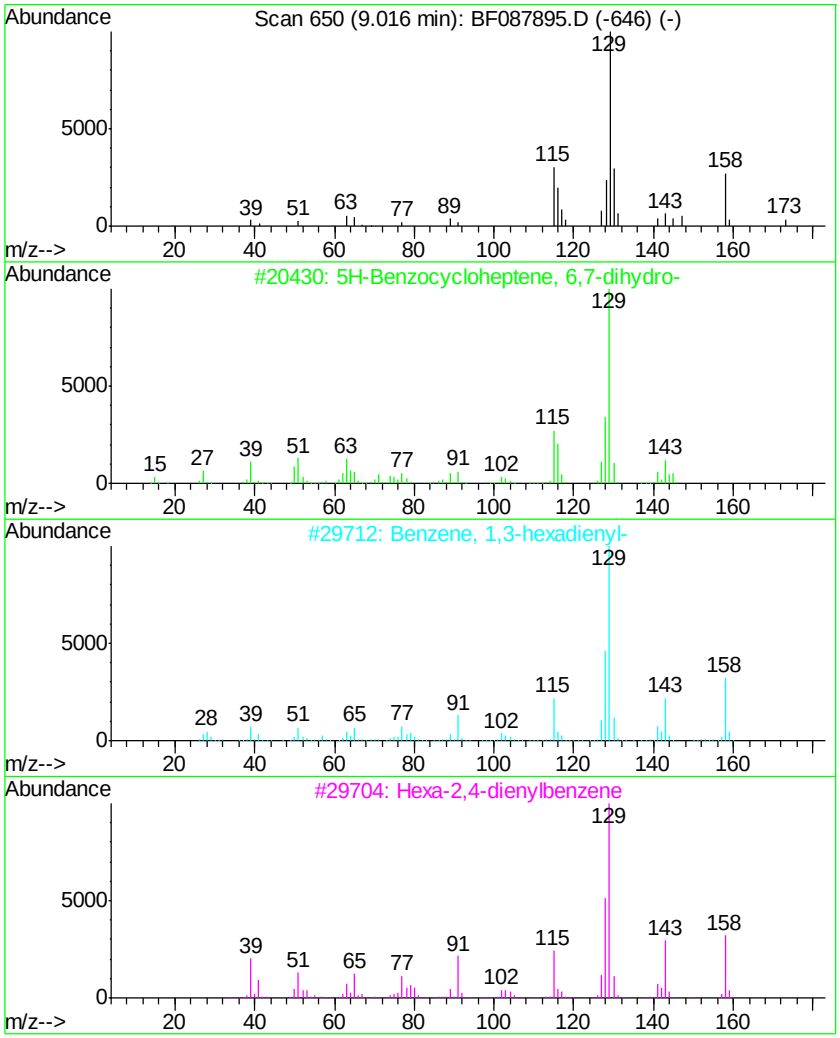
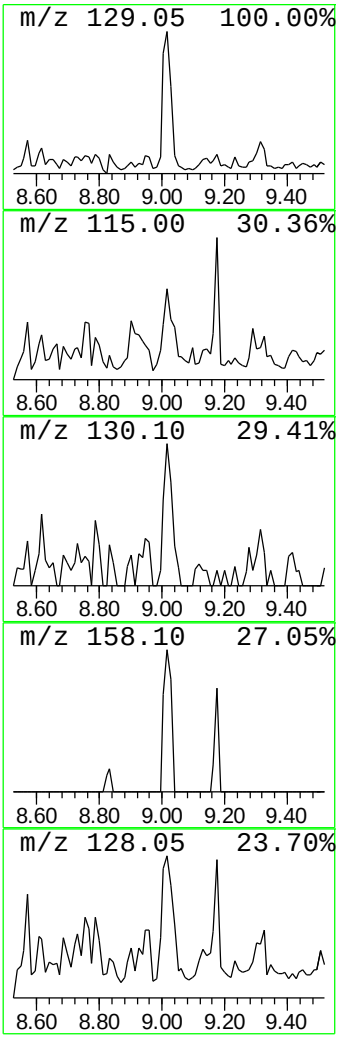
Peak Number 10 5H-Benzocycloheptene, 6,7-d... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	2.14 ng	75341	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	59
2	Benzene, 1,3-hexadienyl-	158	C12H14	041635-77-2	50
3	Hexa-2,4-dienylbenzene	158	C12H14	079482-86-3	28
4	Cyclohexene, 1-phenyl-	158	C12H14	000771-98-2	25
5	1,4-Ethanonaphthalene, 1,2,3,4-t...	158	C12H14	004175-52-4	25





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	2.6	ng	74335	1	6.81	581703	20.0
unknown6.58	6.58	75.9	ng	2207220	1	6.81	581703	20.0
Benzene, 1,2-diet...	7.15	4.0	ng	114946	1	6.81	581703	20.0
Benzene, 1,2,3,4-...	7.59	4.2	ng	171382	2	8.10	821456	20.0
Benzene, (2-methy...	7.75	2.3	ng	93071	2	8.10	821456	20.0
Benzene, 2-etheny...	7.84	11.2	ng	459234	2	8.10	821456	20.0
5H-Benzocyclohept...	9.02	2.1	ng	75341	3	9.85	705334	20.0