LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126390.D
Acq On : 28 Dec 2021 19:49
Operator : JU/CG
Sample : M5239-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-123-1-40-57

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	11	rVB	107575	97701	2.46%	0.396%
2	4.393	388	392	399	rBV	393123	438629	11.05%	1.778%
3	5.022	490	499	508	rBV	987235	1316745	33.17%	5.337%
4	5.428	563	568	571	rBV	3820344	3970259	100.00%	16.092%
5	5.822	632	635	641	rVB	87920	72414	1.82%	0.294%
6	6.439	734	740	743	rBV	2836557	3126933	78.76%	12.674%
7	6.810	799	803	806	rBV	1005474	887730	22.36%	3.598%
8	7.369	893	898	901	rBV	2306290	2398259	60.41%	9.721%
9	8.092	1016	1021	1024	rBV	1157565	1049231	26.43%	4.253%
10	9.169	1199	1204	1208	rBV	3594476	3449814	86.89%	13.983%
11	9.845	1315	1319	1326	rBV	1494826	1275647	32.13%	5.170%
12	10.263	1386	1390	1393	rBV2	118799	114411	2.88%	0.464%
13	10.633	1449	1453	1461	rBV	2028218	1872414	47.16%	7.589%
14	11.333	1568	1572	1578	rBV	984570	961116	24.21%	3.896%
15	11.863	1659	1662	1665	rBV	49807	49747	1.25%	0.202%
16	12.921	1837	1842	1845	rBV	2426102	2211670	55.71%	8.964%
17	13.863	1997	2002	2016	rBV6	41774	133174	3.35%	0.540%
18	13.968	2016	2020	2029	rVB	688269	635421	16.00%	2.575%
19	14.827	2162	2166	2172	rVB	61170	63010	1.59%	0.255%
20	15.415	2261	2266	2272	rBV2	412156	547478	13.79%	2.219%

Sum of corrected areas: 24671803

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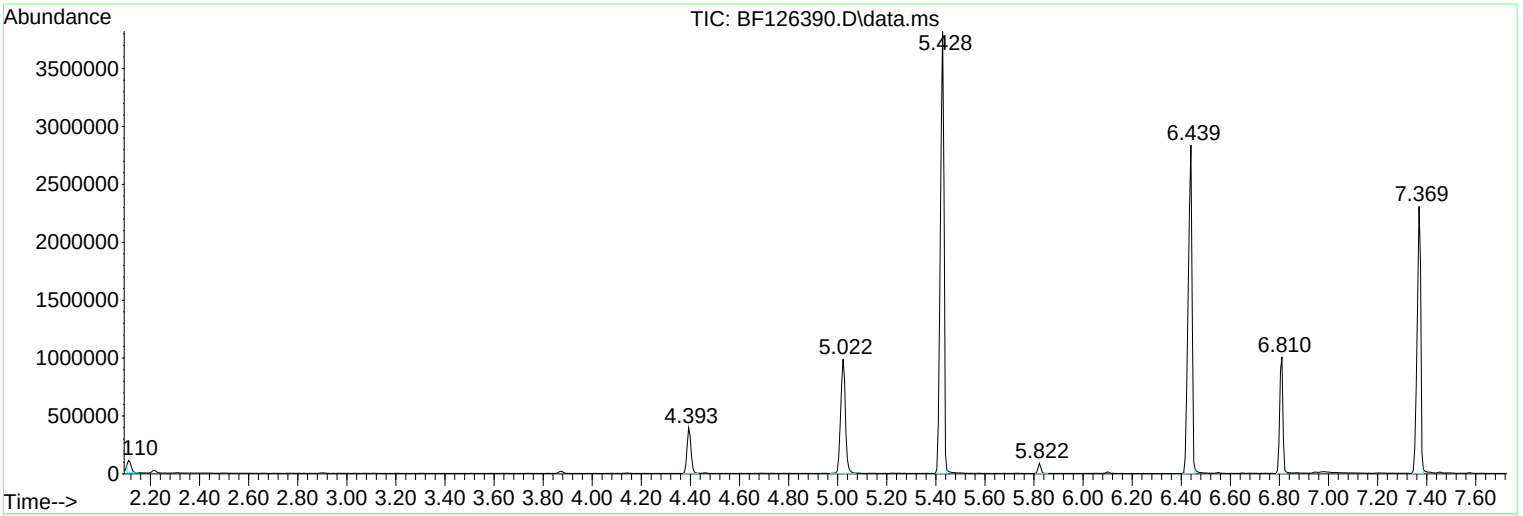
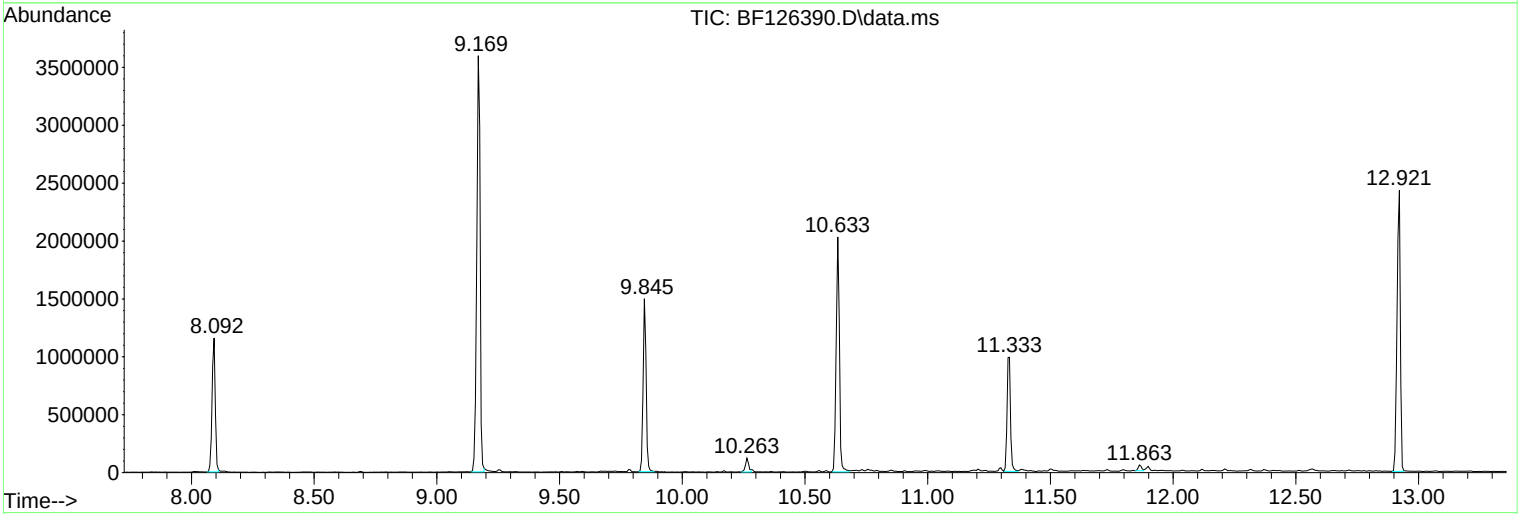
Misc :
ALS Vial : 14 Sample Multiplier: 1

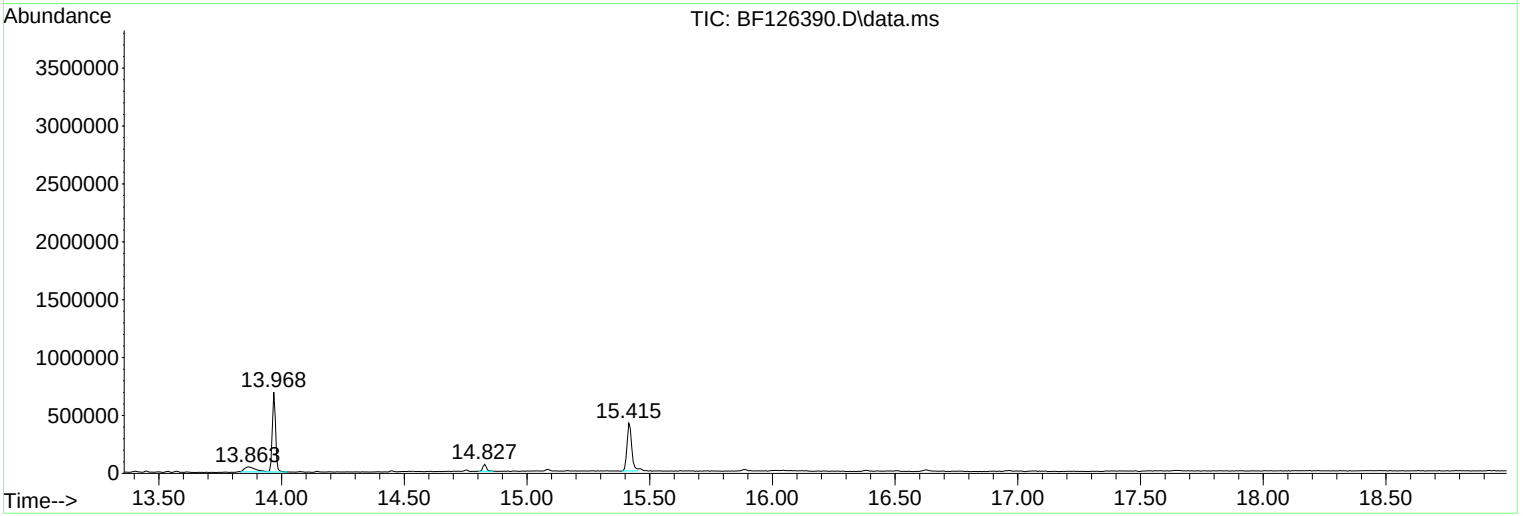
Instrument :
BNA_F
ClientSampleId :
SASP2-123-1-40-57

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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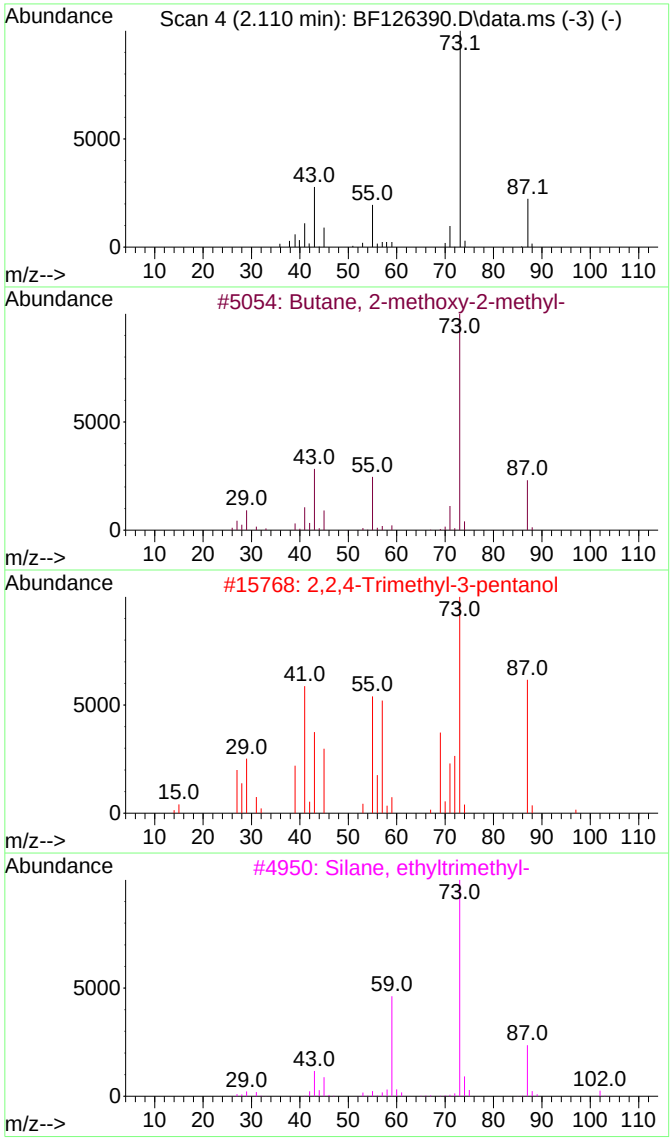
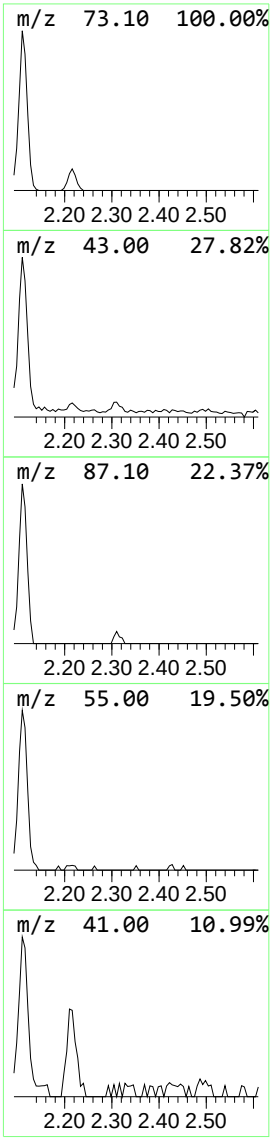
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.110	2.20 ng	97701	1,4-Dichlorobenzene-d4	6.810

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	74
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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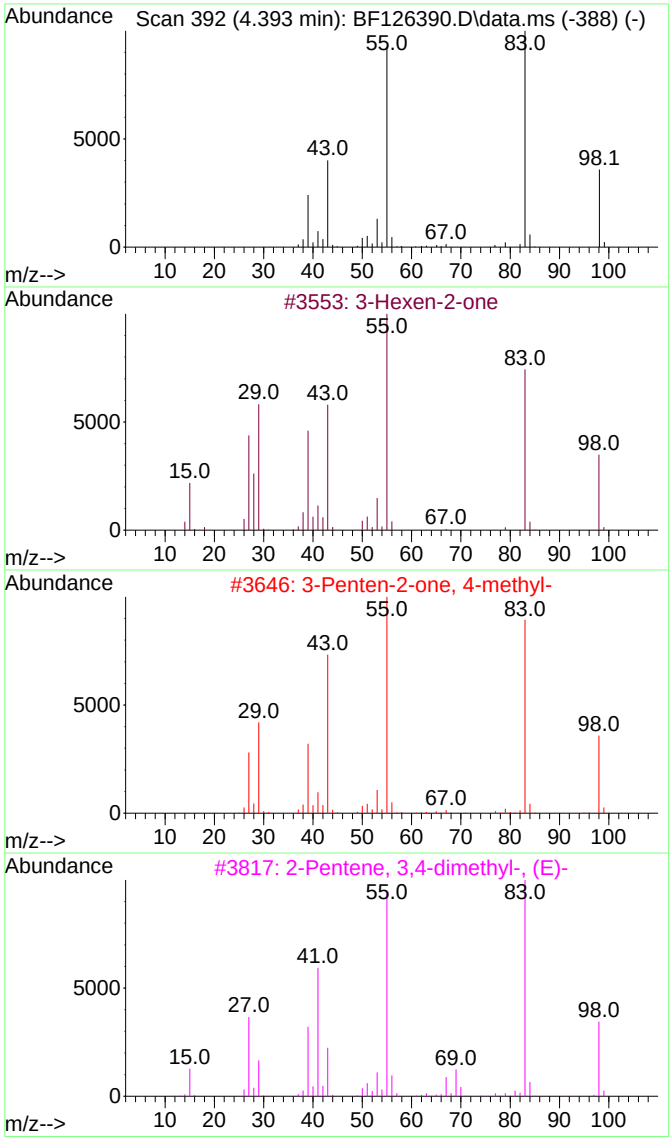
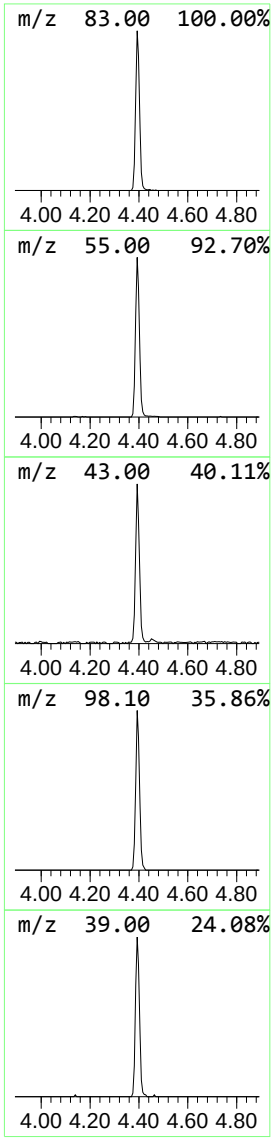
Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.393	9.88 ng	438629	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80





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Data File : BF126390.D
Acq On : 28 Dec 2021 19:49
Operator : JU/CG
Sample : M5239-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-123-1-40-57

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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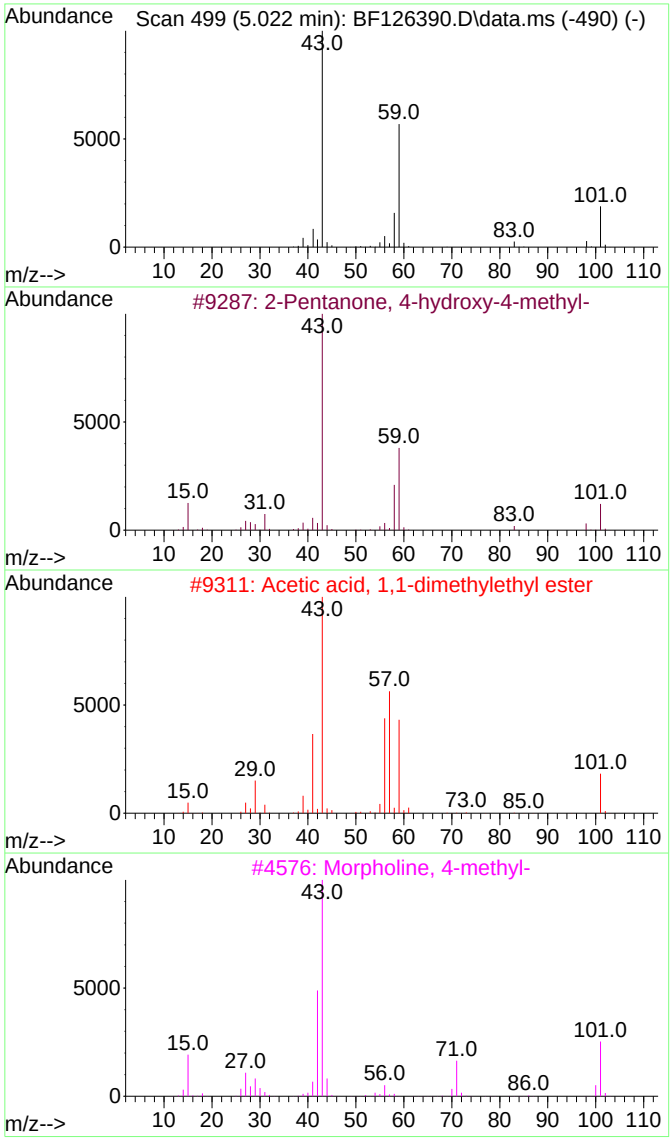
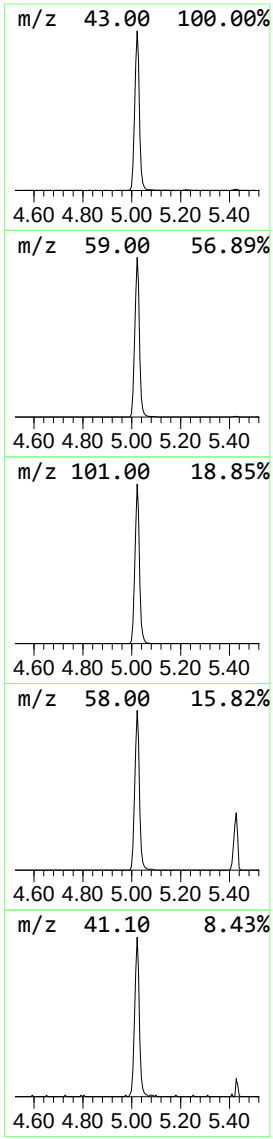
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	29.67 ng	1316750	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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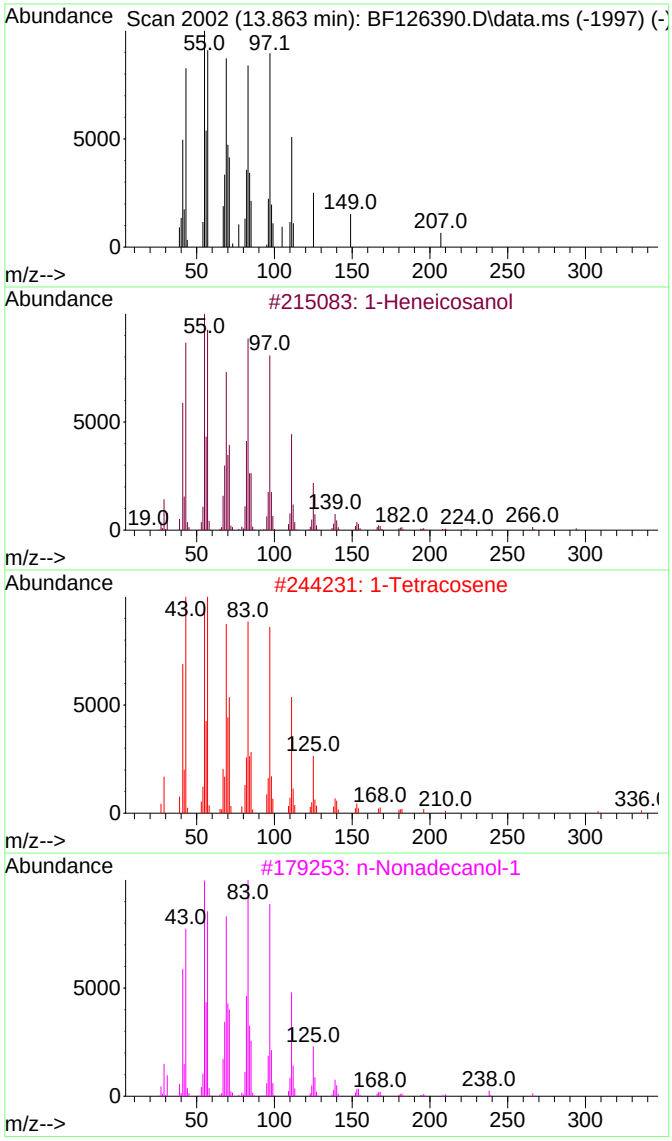
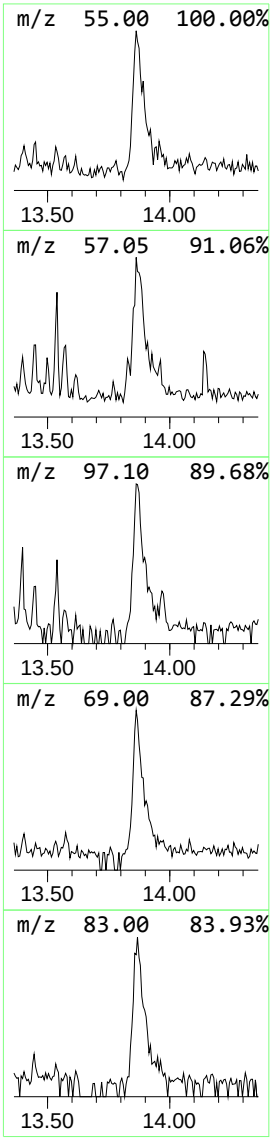
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	4.19 ng	133174	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Sample : M5239-04
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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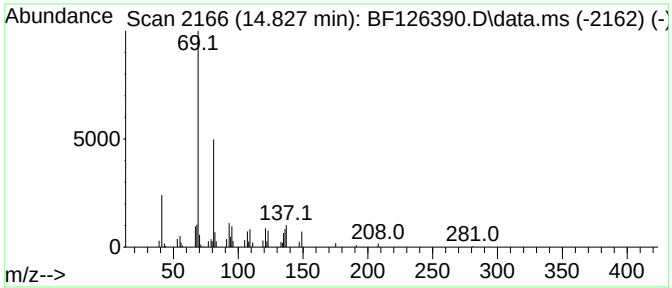
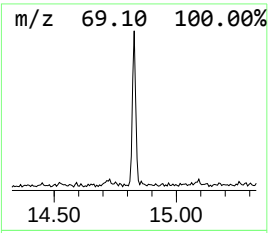
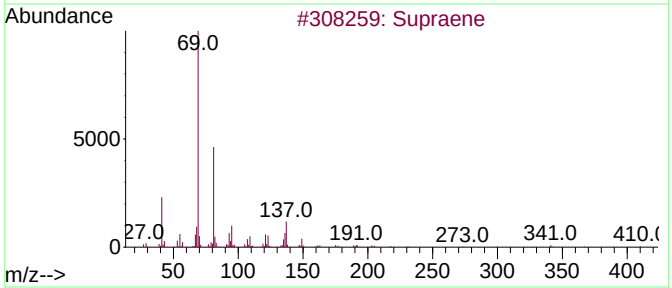
Peak Number 5 Supraene Concentration Rank 4

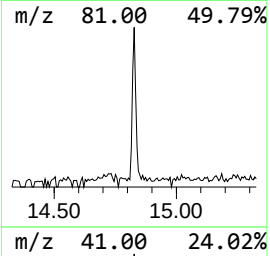
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	2.30 ng	63010	Perylene-d12	15.415

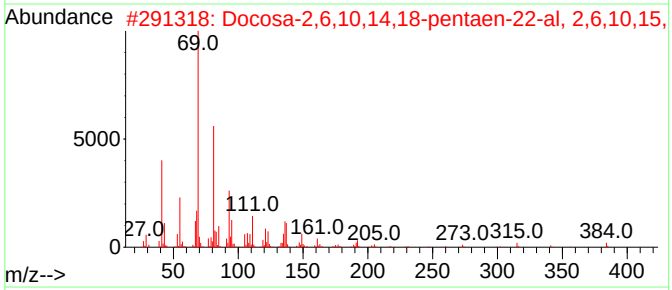
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
4	trans-Farnesol	222	C15H26O	000106-28-5	72
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72

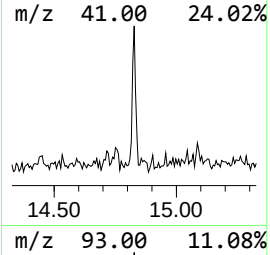


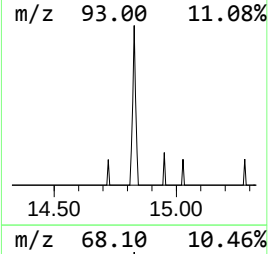


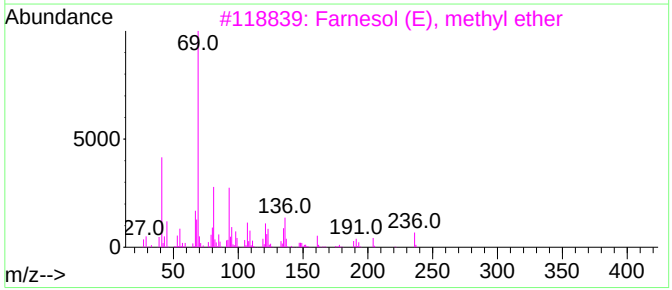


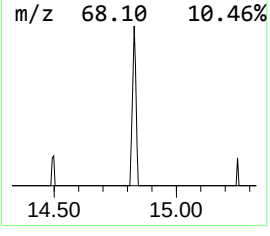












Tentatively Identified Compound (LSC) summary

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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...	2.110	2.2	ng	97701	1	6.810	887730	20.0
3-Hexen-2-one	4.393	9.9	ng	438629	1	6.810	887730	20.0
2-Pentanone, 4-...	5.022	29.7	ng	1316750	1	6.810	887730	20.0
1-Heneicosanol	13.863	4.2	ng	133174	5	13.968	635421	20.0
Supraene	14.827	2.3	ng	63010	6	15.415	547478	20.0