LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
Data File : BF136134.D
Acq On : 03 Nov 2023 20:11
Operator : CG\JU
Sample : 05214-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-221

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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	507	rBV	42309	50084	3.28%	0.391%
2	5.446	566	571	574	rBV	1580335	1368245	89.60%	10.693%
3	6.445	736	741	744	rBV	1381448	1349658	88.39%	10.548%
4	6.816	801	804	808	rBV	605896	478841	31.36%	3.742%
5	7.375	895	899	902	rBV	950316	867400	56.80%	6.779%
6	8.098	1018	1022	1025	rBV	804056	608925	39.88%	4.759%
7	9.175	1202	1205	1208	rBV	1991174	1526982	100.00%	11.934%
8	9.292	1223	1225	1229	rVB	41783	35948	2.35%	0.281%
9	9.492	1255	1259	1260	rBV	28218	24642	1.61%	0.193%
10	9.516	1260	1263	1266	rVB	339807	280091	18.34%	2.189%
11	9.769	1302	1306	1308	rBV2	23384	20018	1.31%	0.156%
12	9.833	1313	1317	1318	rVV	110507	91284	5.98%	0.713%
13	9.857	1318	1321	1324	rVV	780517	637039	41.72%	4.979%
14	9.886	1324	1326	1332	rVB	43572	38443	2.52%	0.300%
15	9.981	1338	1342	1346	rBV	41911	33824	2.22%	0.264%
16	10.645	1449	1455	1458	rBV	1068221	877564	57.47%	6.858%
17	11.345	1570	1574	1577	rBV	679277	562807	36.86%	4.398%
18	11.369	1577	1578	1582	rVB	57762	35341	2.31%	0.276%
19	11.886	1662	1666	1670	rBV	64298	68261	4.47%	0.533%
20	12.563	1778	1781	1785	rBV	143678	130384	8.54%	1.019%
21	12.674	1796	1800	1812	rBV5	15091	28981	1.90%	0.226%
22	12.792	1814	1820	1825	rBV2	111694	116686	7.64%	0.912%
23	12.945	1842	1846	1850	rBV	1511298	1238904	81.13%	9.682%
24	13.380	1918	1920	1924	rBV2	21154	20349	1.33%	0.159%
25	13.421	1924	1927	1937	rVB6	24614	29558	1.94%	0.231%
26	13.721	1974	1978	1981	rBV	609189	471251	30.86%	3.683%
27	13.898	2001	2008	2009	rBV7	17166	28739	1.88%	0.225%
28	14.004	2021	2026	2029	rBV	585413	560540	36.71%	4.381%
29	14.027	2029	2030	2032	rVB	64278	31527	2.06%	0.246%
30	14.498	2103	2110	2112	rBV4	19849	29943	1.96%	0.234%
31	14.598	2124	2127	2133	rVB4	26042	45587	2.99%	0.356%
32	14.651	2133	2136	2141	rBV	95769	110160	7.21%	0.861%
33	14.792	2155	2160	2166	rVB4	41444	95562	6.26%	0.747%
34	14.957	2185	2188	2192	rVB3	36171	37297	2.44%	0.291%
35	14.992	2192	2194	2199	rVB2	19400	21826	1.43%	0.171%
36	15.051	2199	2204	2207	rBV2	53003	79389	5.20%	0.620%

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Instrument :
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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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.163	2219	2223	2227	rVB	24524	29707	1.95%	0.232%
38	15.363	2253	2257	2263	rVB	27198	35733	2.34%	0.279%
39	15.421	2263	2267	2271	rVB	27819	35046	2.30%	0.274%
40	15.492	2273	2279	2287	rVV	468001	567708	37.18%	4.437%
41	16.021	2364	2369	2376	rBV2	18515	32794	2.15%	0.256%
42	16.986	2528	2533	2538	rBV2	10805	20469	1.34%	0.160%
43	17.192	2563	2568	2574	rVB8	10635	20547	1.35%	0.161%
44	17.451	2606	2612	2618	rVB3	8111	21605	1.41%	0.169%

Sum of corrected areas: 12795689

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Instrument :
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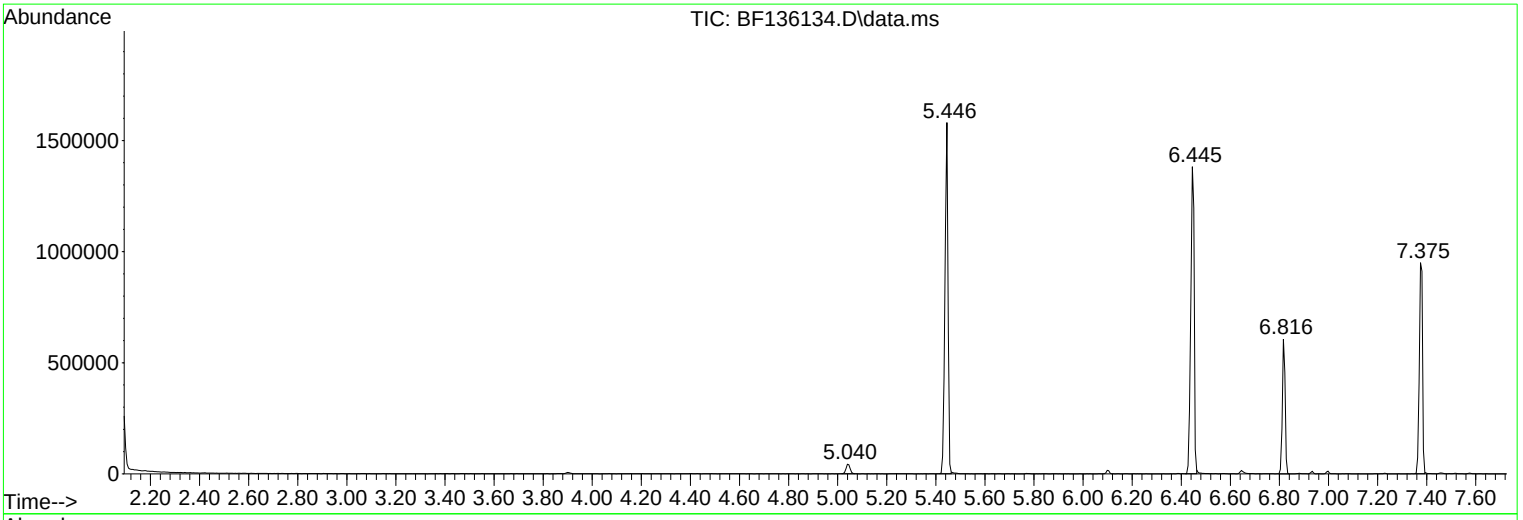
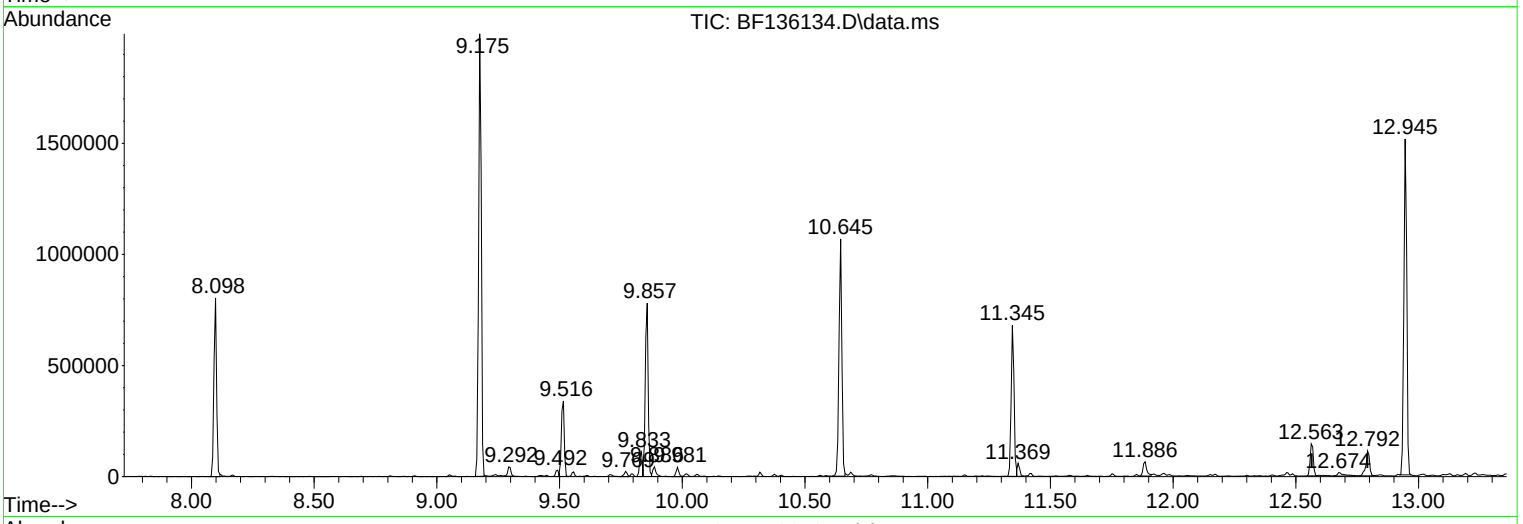
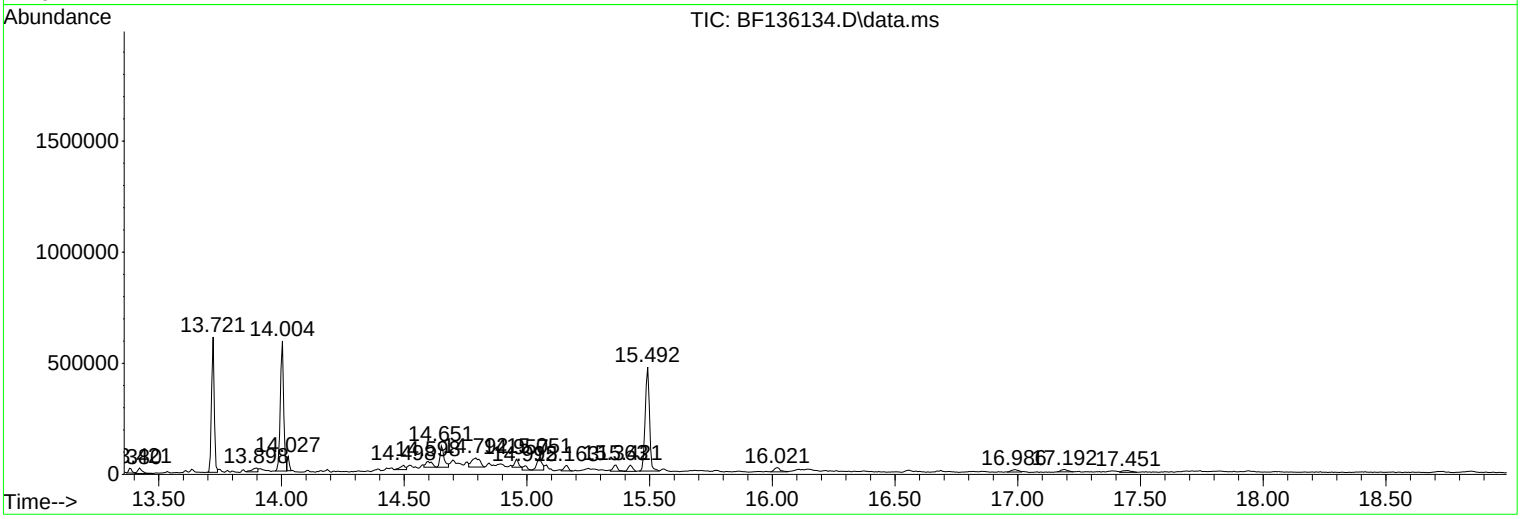
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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ALS Vial : 21 Sample Multiplier: 1

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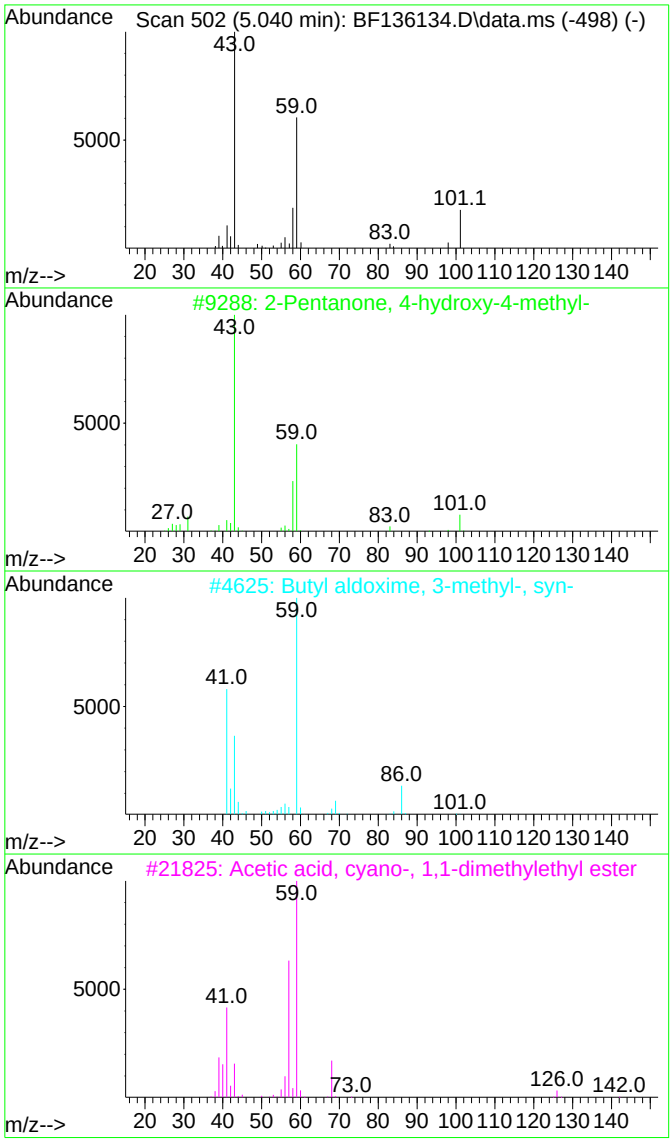
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

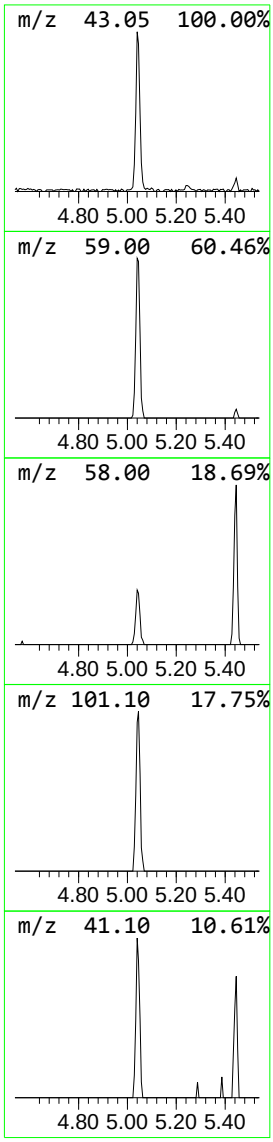
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.09 ng	50084	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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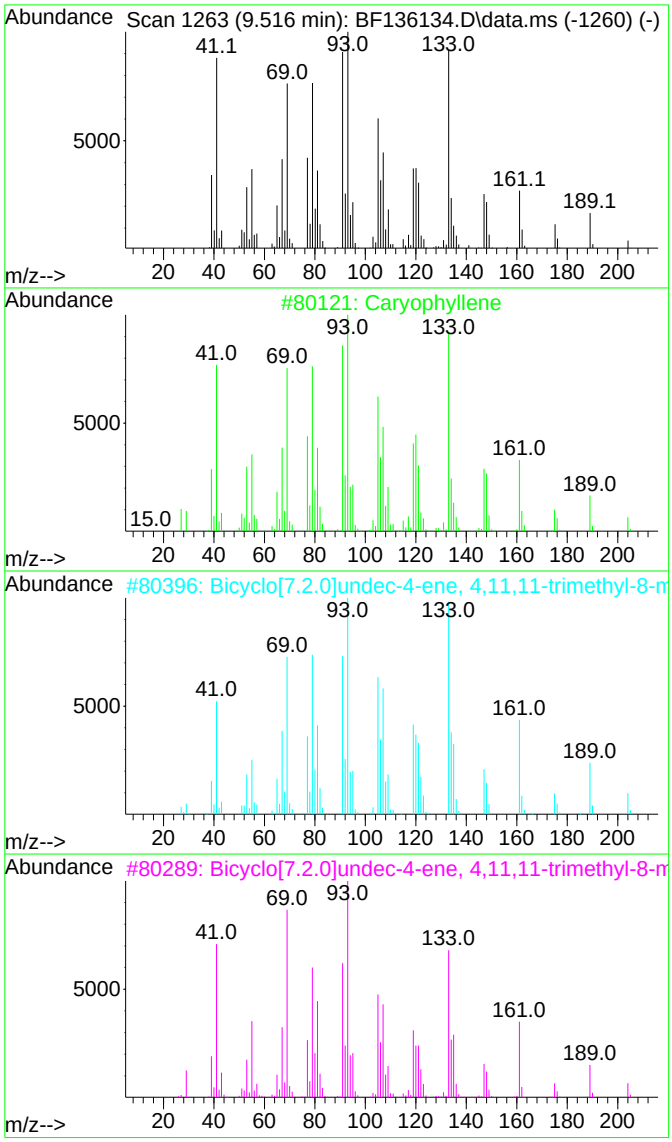
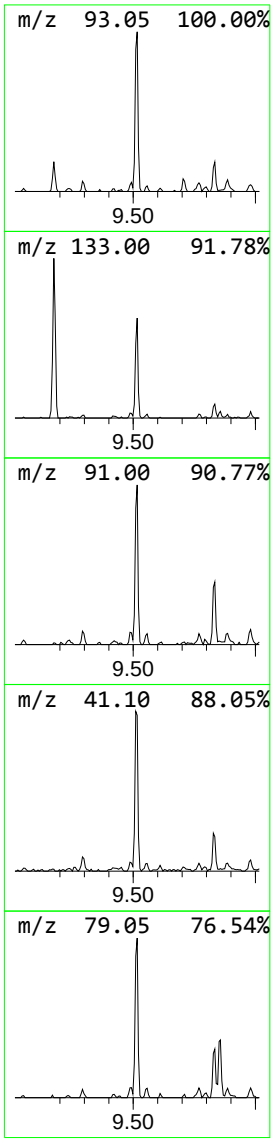
Peak Number 2 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.516	8.79 ng	280091	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	93
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	89
4	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	58
5	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	45





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Data File : BF136134.D
Acq On : 03 Nov 2023 20:11
Operator : CG\JU
Sample : 05214-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

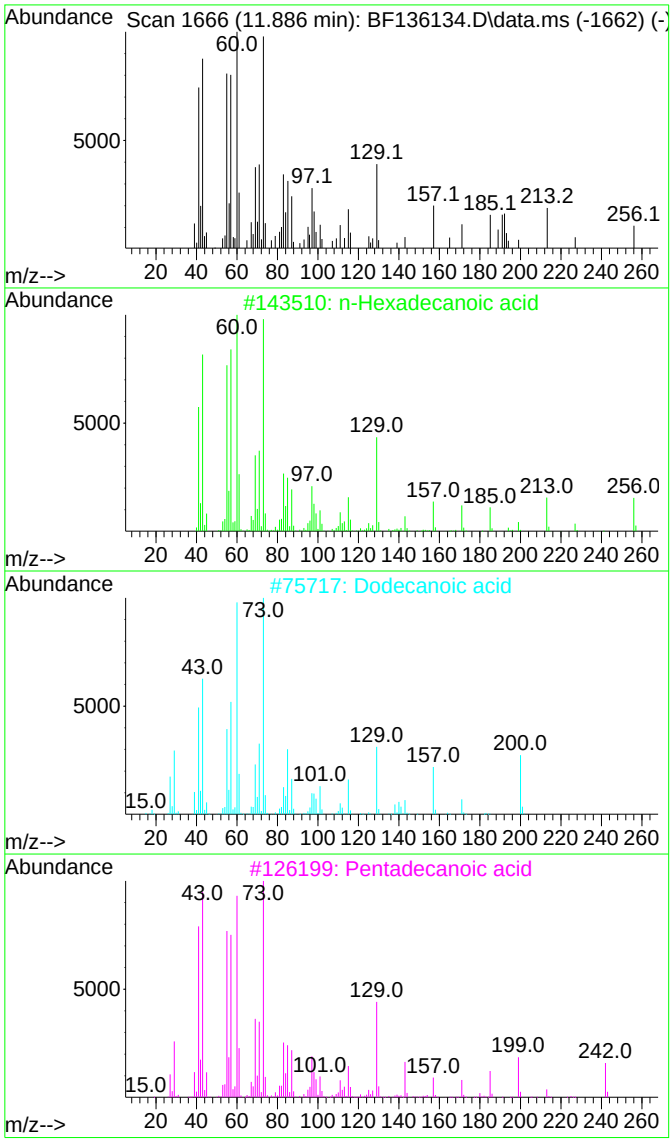
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

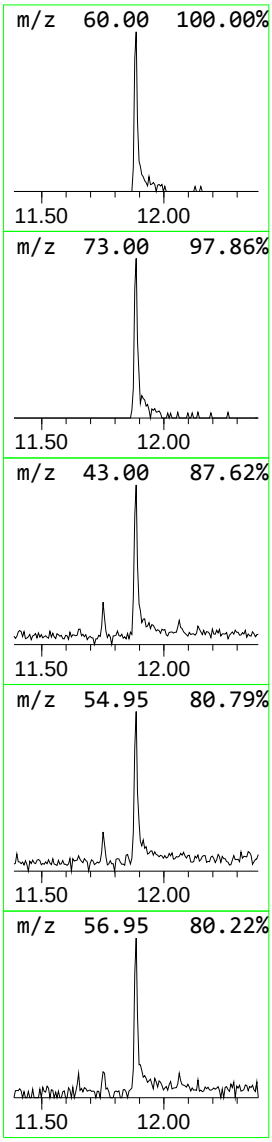
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.43 ng	68261	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Dodecanoic acid	200	C12H24O2	000143-07-7	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Butyl dodecyl ether	242	C16H34O	1000406-40-3	22
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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BNA_F
ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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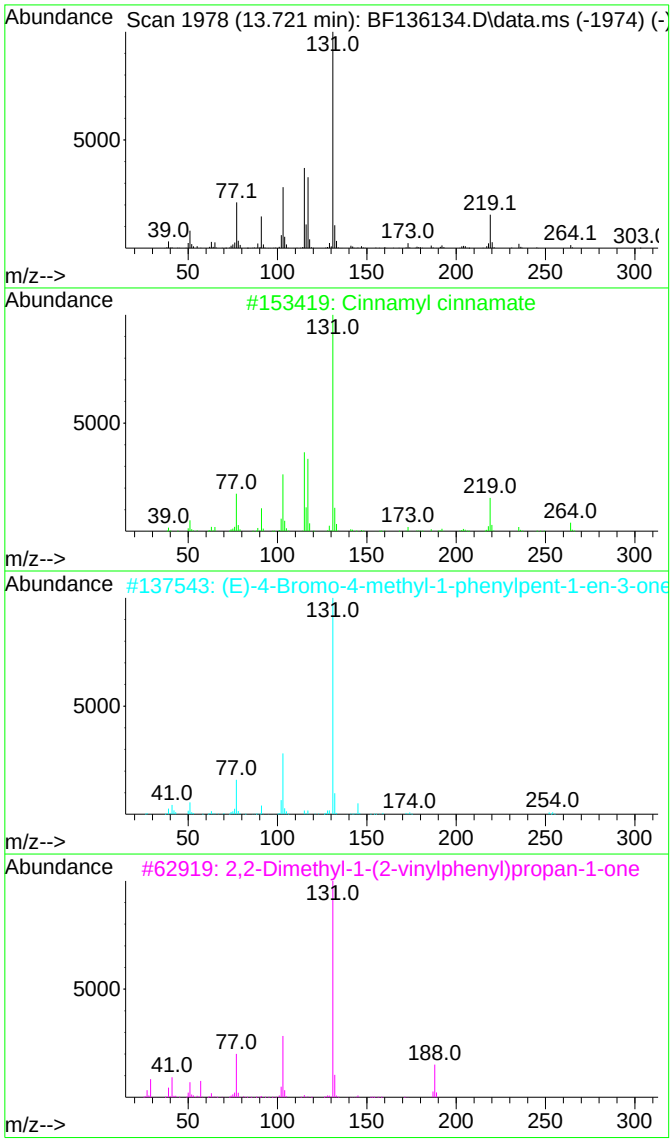
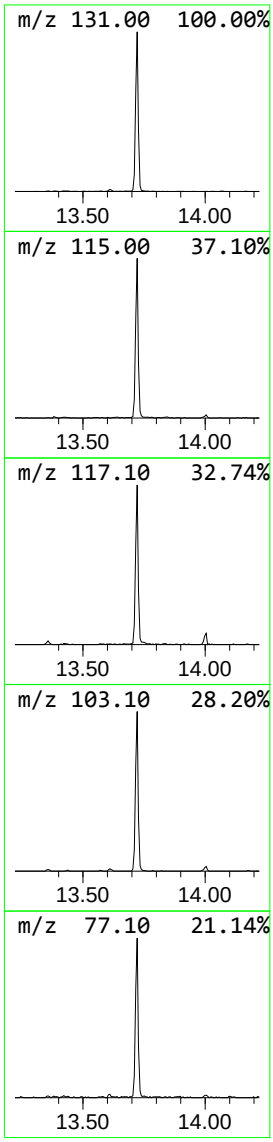
Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.721	16.81 ng	471251	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	53
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
4	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	50
5	Oxalic acid, monoamide monohydra...	323	C18H17N3O3	1000294-01-4	50





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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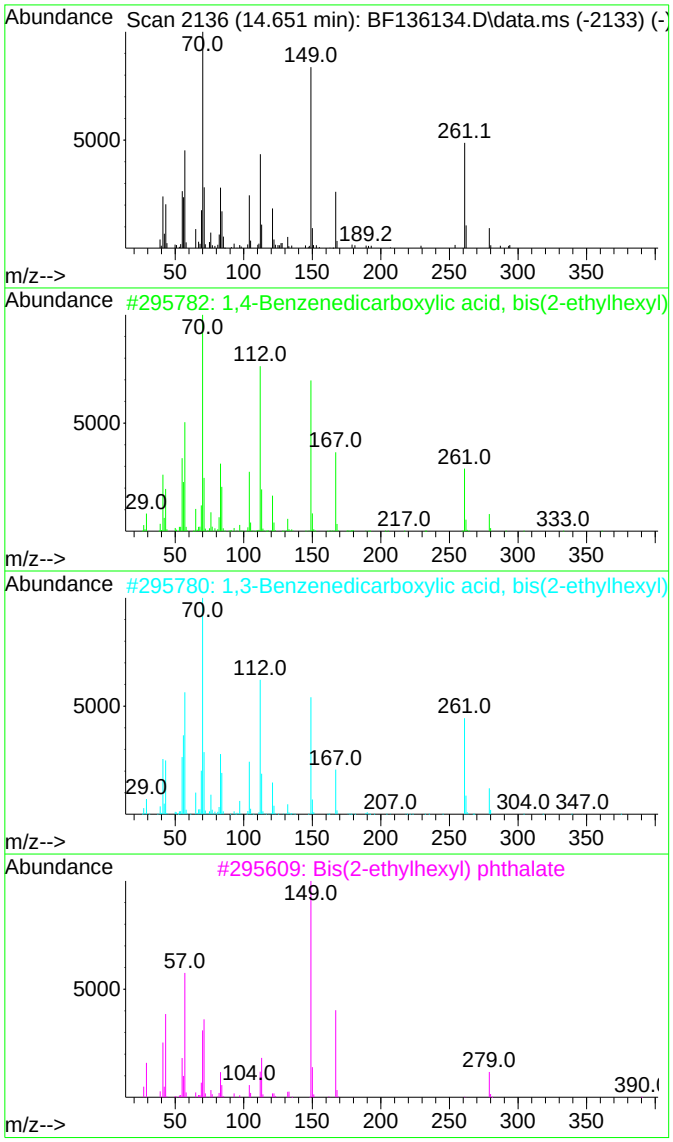
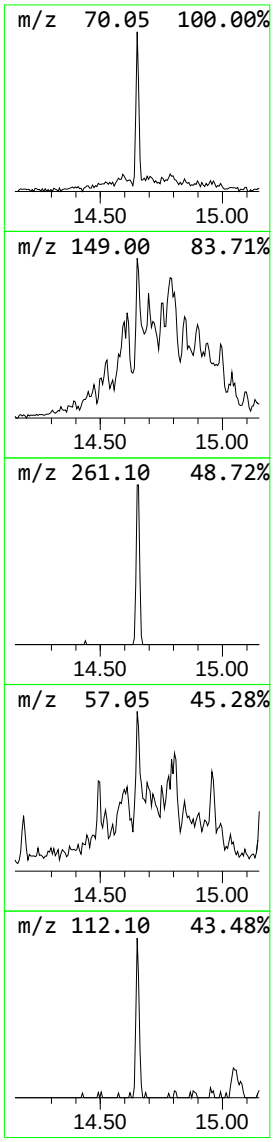
Peak Number 5 unknown14.651 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	3.93 ng	110160	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	49
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	46
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	35
4	Di(Z)-hex-3-enyl phthalate	330	C20H26O4	1000373-65-0	22
5	1,4-benzenedicarboxylic acid, mo...	208	C11H12O4	1000400-56-6	22





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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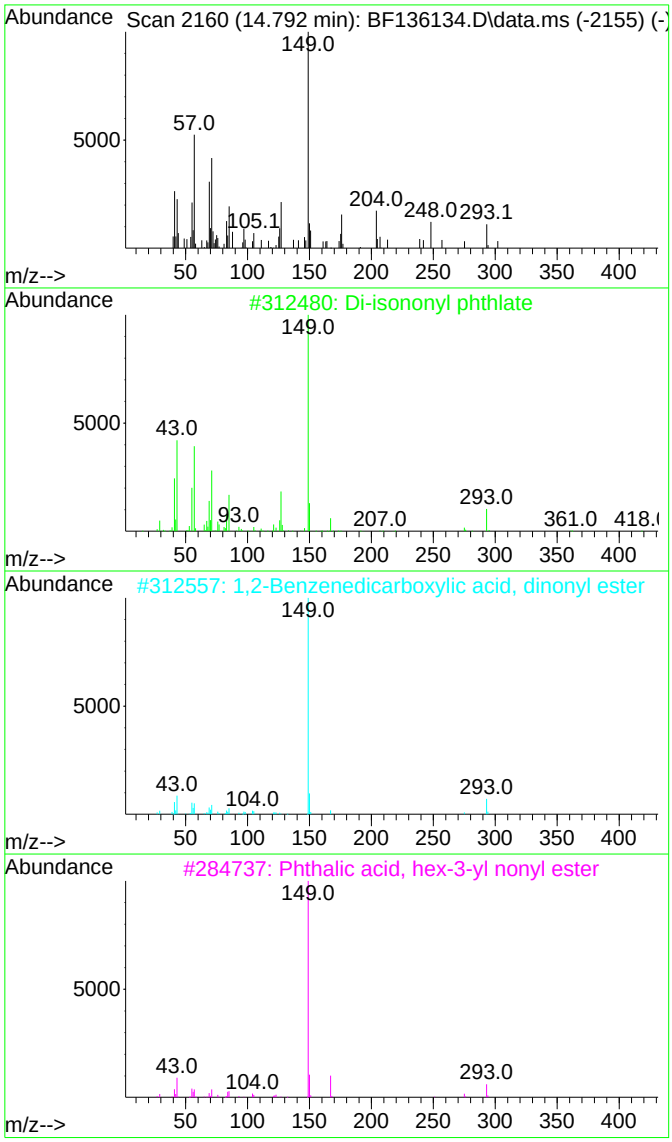
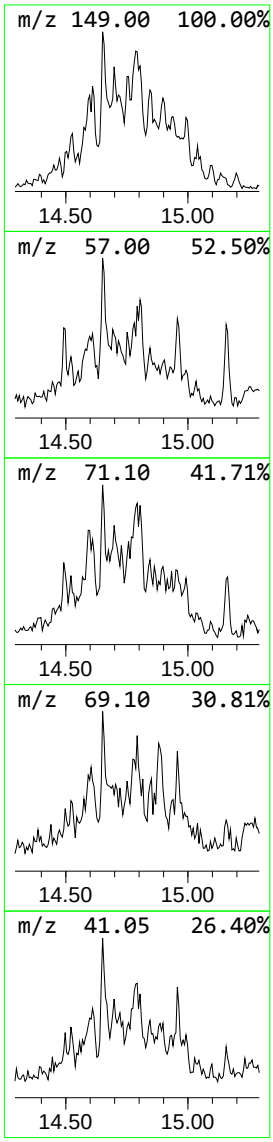
Peak Number 6 Di-isononyl phthlate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	3.37 ng	95562	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-isononyl phthlate	418	C26H42O4	020548-62-3	64
2	1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	38
3	Phthalic acid, hex-3-yl nonyl ester	376	C23H36O4	1000356-96-0	35
4	Phthalic acid, nonyl trans-hex-3...	374	C23H34O4	1000360-48-7	35
5	Phthalic acid, 5-methoxy-3-methy...	406	C24H38O5	1000315-38-1	35





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	2.1	ng	50084	1	6.816	478841	20.0
Caryophyllene	9.516	8.8	ng	280091	3	9.857	637039	20.0
n-Hexadecanoic ...	11.886	2.4	ng	68261	4	11.345	562807	20.0
Cinnamyl cinnamate	13.721	16.8	ng	471251	5	14.004	560540	20.0
unknown14.651	14.651	3.9	ng	110160	5	14.004	560540	20.0
Di-isononyl pht...	14.792	3.4	ng	95562	6	15.492	567708	20.0