

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
 Data File : BF126302.D
 Acq On : 21 Dec 2021 18:10
 Operator : JU/CG
 Sample : M5018-69
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP9

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: BF126302.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	15	rVB	668673	808861	17.39%	2.222%
2	5.034	492	501	516	rBV	624030	863767	18.58%	2.373%
3	5.434	564	569	572	rBV	3923221	4098956	88.15%	11.259%
4	5.828	633	636	644	rVB	65119	62742	1.35%	0.172%
5	6.445	735	741	744	rBV	3685525	4338637	93.30%	11.917%
6	6.816	800	804	807	rBV	1481835	1219203	26.22%	3.349%
7	7.375	894	899	903	rBV	2510468	2972556	63.93%	8.165%
8	8.098	1017	1022	1039	rVB	1816343	1742682	37.48%	4.787%
9	8.698	1120	1124	1125	rBV	51175	56172	1.21%	0.154%
10	8.716	1125	1127	1131	rVB	373698	308174	6.63%	0.846%
11	9.174	1200	1205	1217	rBV	3971021	4649992	100.00%	12.773%
12	9.263	1217	1220	1228	rVB2	105985	131734	2.83%	0.362%
13	9.492	1256	1259	1261	rBV2	59042	53107	1.14%	0.146%
14	9.792	1306	1310	1314	rVB2	50925	52091	1.12%	0.143%
15	9.851	1315	1320	1332	rBV	1777036	1882916	40.49%	5.172%
16	10.639	1449	1454	1465	rBV	2498869	2764921	59.46%	7.595%
17	10.774	1473	1477	1480	rVB4	45783	57251	1.23%	0.157%
18	11.298	1562	1566	1569	rBV3	63786	74338	1.60%	0.204%
19	11.339	1569	1573	1576	rVV	2016818	1815746	39.05%	4.987%
20	11.868	1660	1663	1666	rBV	135194	120927	2.60%	0.332%
21	12.139	1704	1709	1715	rVB5	41145	76835	1.65%	0.211%
22	12.751	1810	1813	1816	rBV	89959	81793	1.76%	0.225%
23	12.927	1838	1843	1846	rBV	4089826	4087791	87.91%	11.228%
24	13.457	1929	1933	1936	rBV	70987	61348	1.32%	0.169%
25	13.921	2002	2012	2017	rBV2	202432	596605	12.83%	1.639%
26	13.974	2017	2021	2033	rVV	1490141	1652614	35.54%	4.539%
27	14.068	2034	2037	2042	rVB	52612	62102	1.34%	0.171%
28	14.580	2116	2124	2140	rBV4	61772	255308	5.49%	0.701%
29	15.092	2207	2211	2218	rVB	83026	93394	2.01%	0.257%
30	15.421	2262	2267	2272	rBV	797280	1050943	22.60%	2.887%
31	15.462	2272	2274	2280	rVB	66724	86922	1.87%	0.239%
32	15.892	2342	2347	2354	rBV	71160	108297	2.33%	0.297%
33	16.392	2427	2432	2439	rBV2	33223	56742	1.22%	0.156%
34	16.980	2525	2532	2539	rBV4	29433	60503	1.30%	0.166%

Sum of corrected areas: 36405970

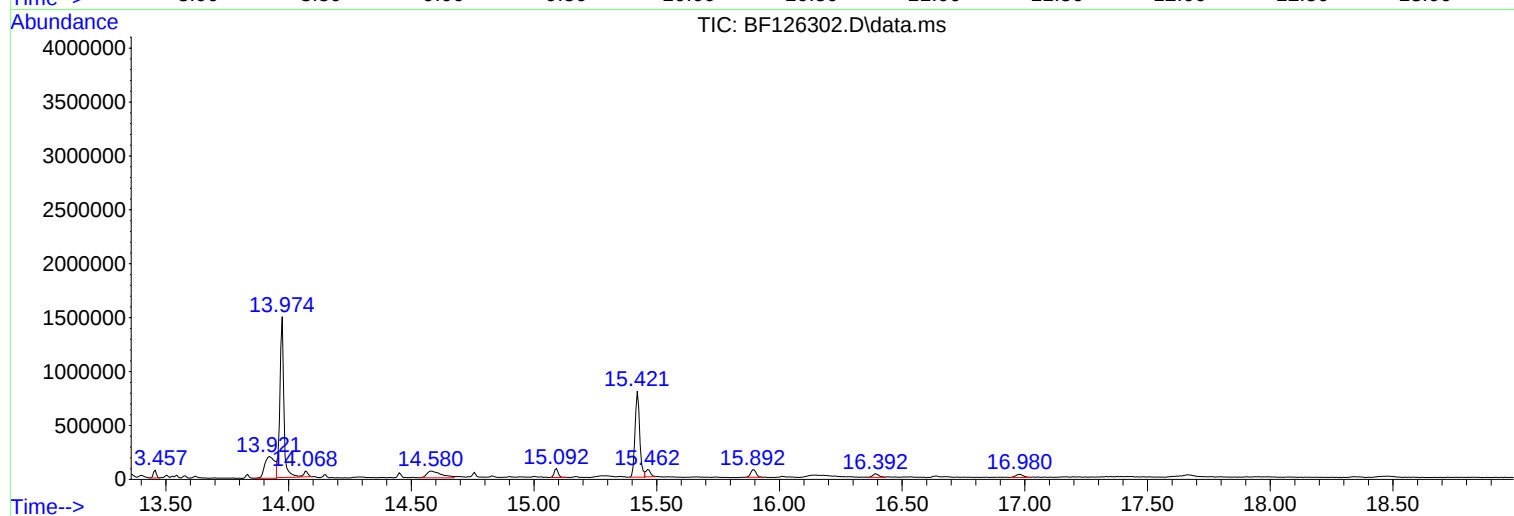
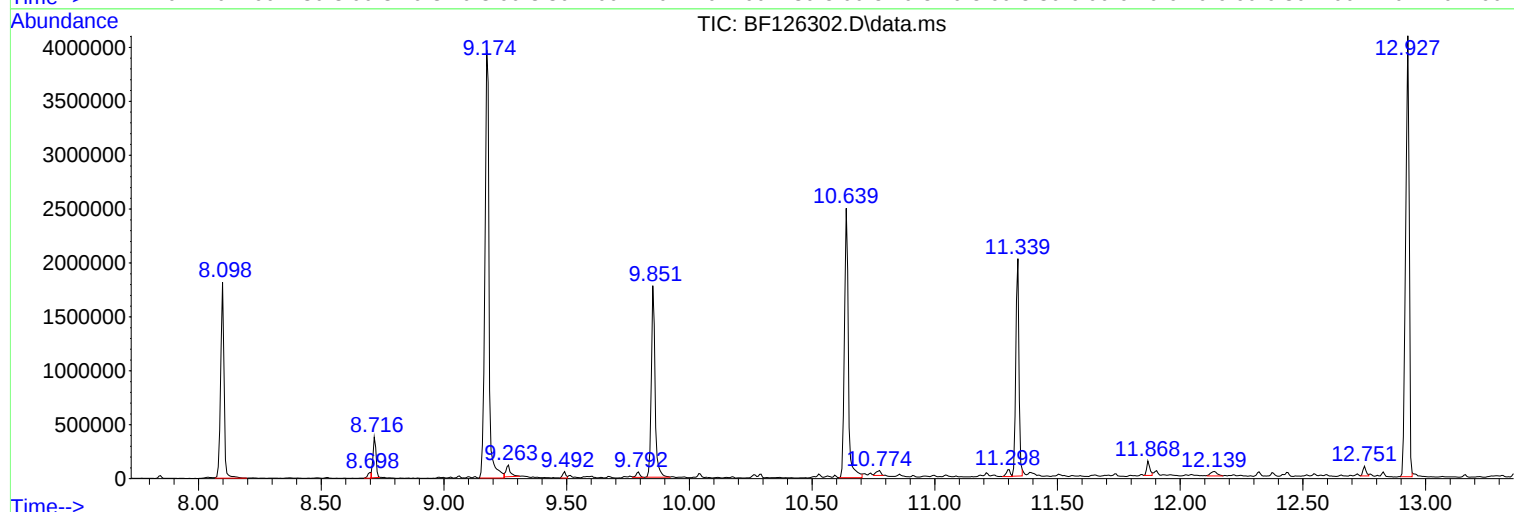
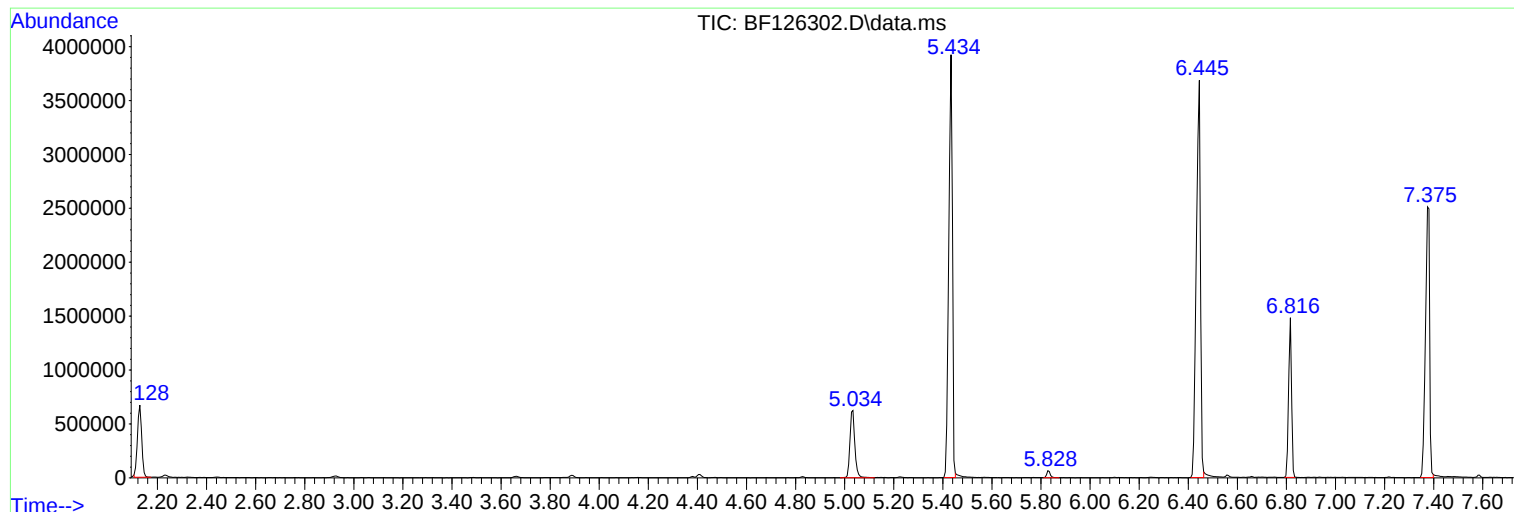
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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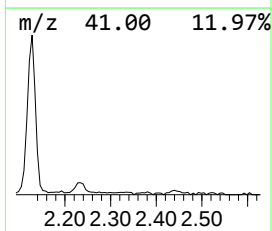
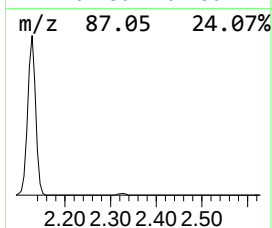
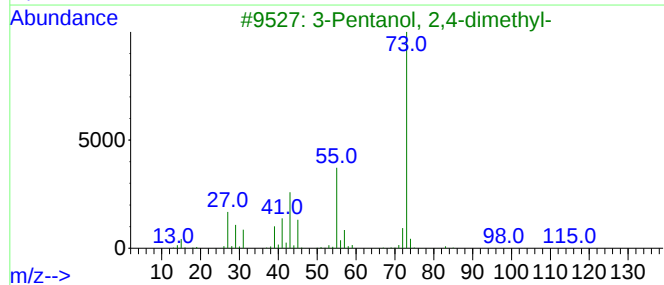
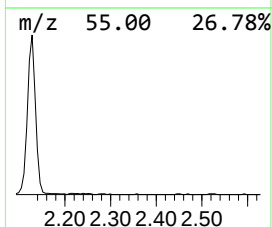
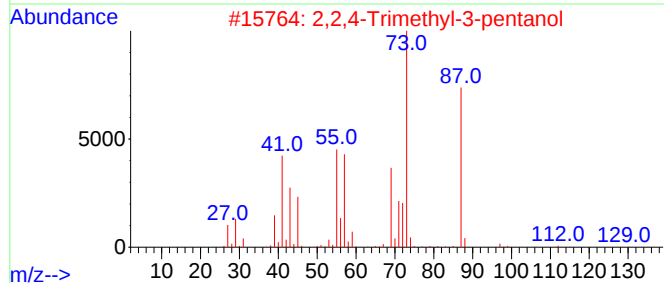
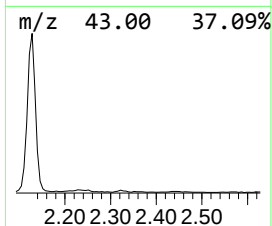
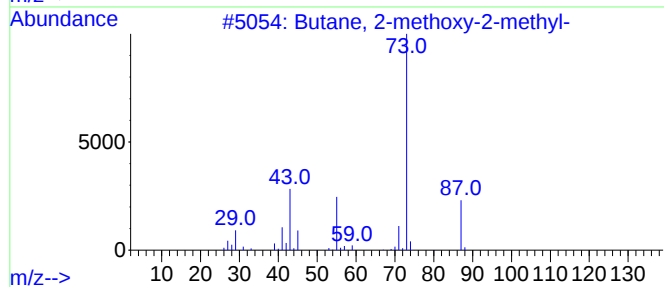
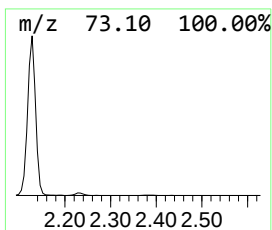
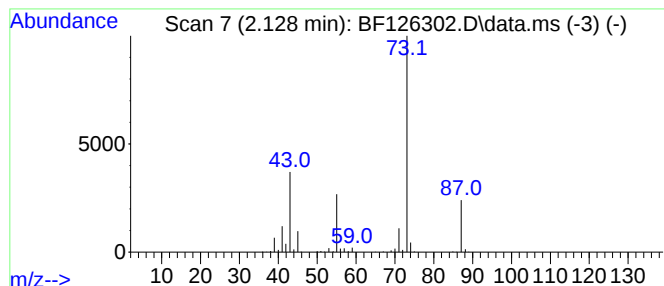
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	13.27 ng	808861	1,4-Dichlorobenzene-d4	6.816

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	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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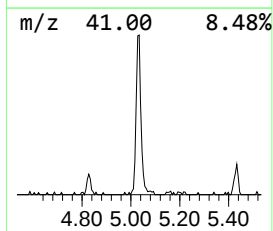
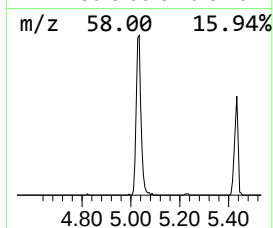
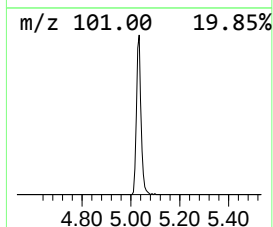
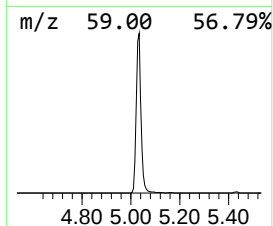
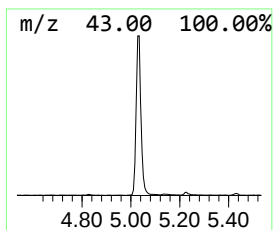
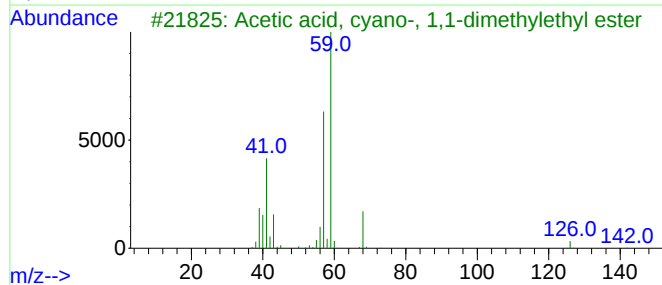
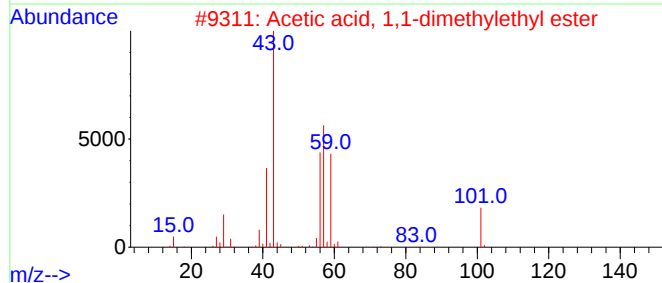
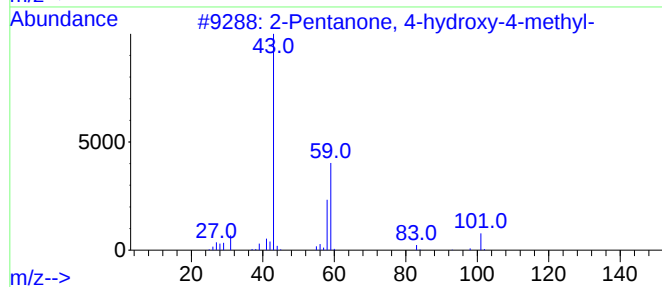
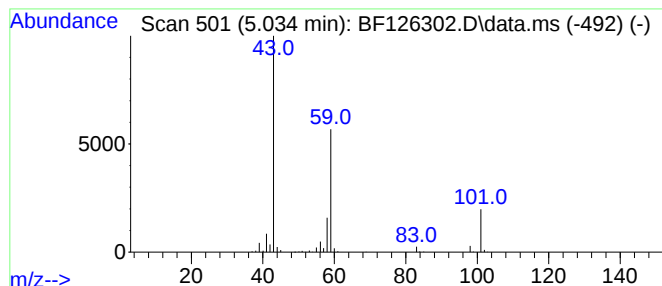
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	14.17 ng	863767	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	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Acetone	58	C3H6O	000067-64-1	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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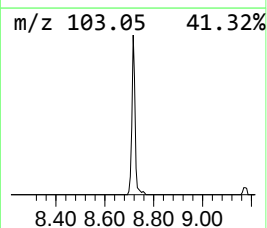
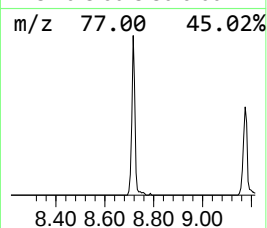
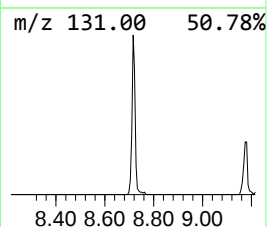
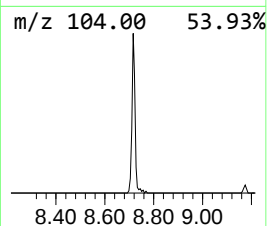
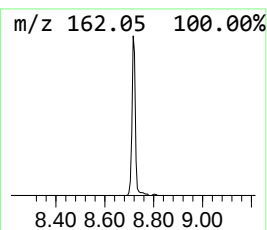
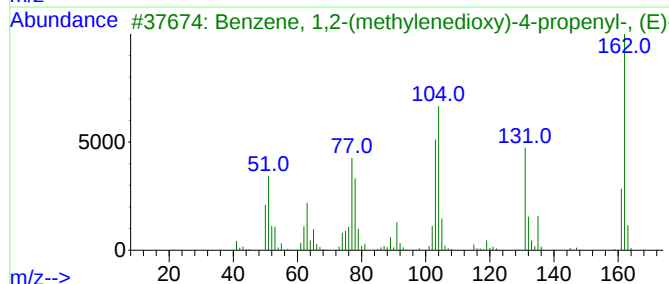
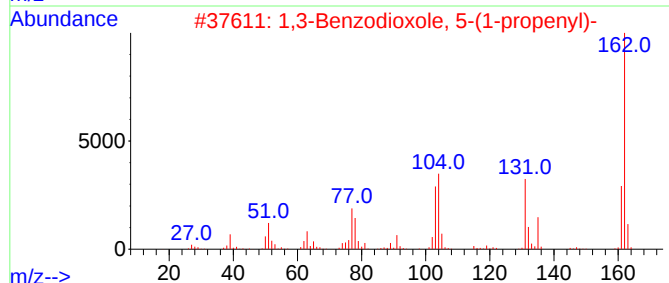
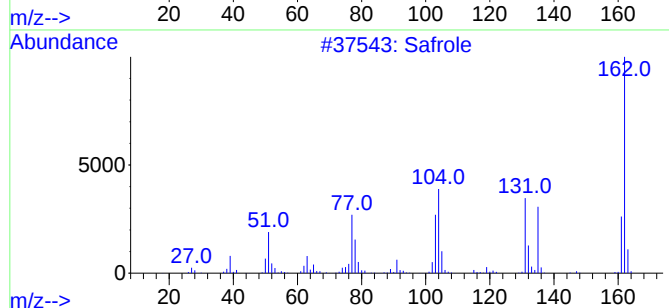
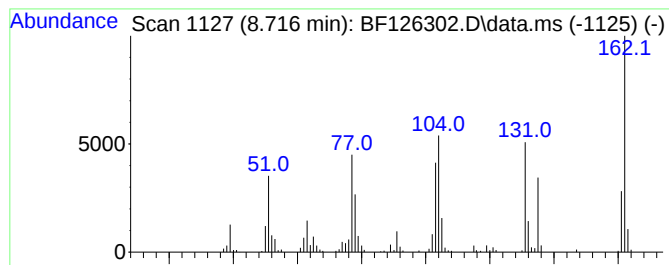
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Peak Number 3 Safole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.716	3.54 ng	308174	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Safole	162	C10H10O2	000094-59-7	98
2			1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	94
3			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	91
4			1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	50
5			(Z)-3-Phenylacrylaldehyde	132	C9H8O	057194-69-1	50



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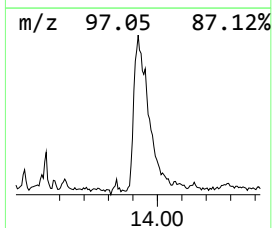
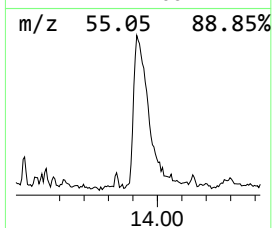
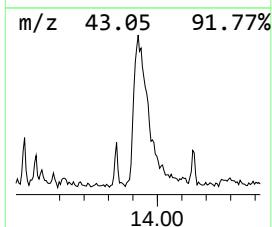
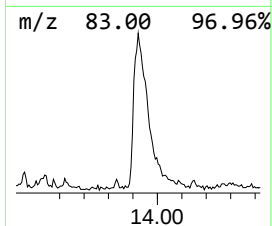
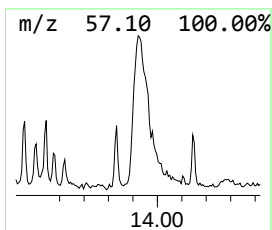
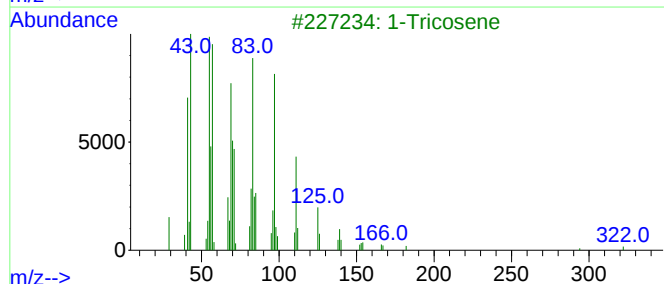
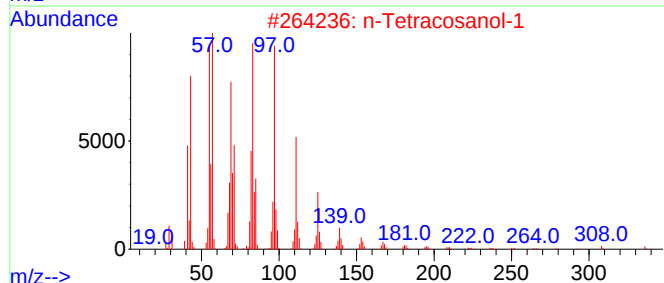
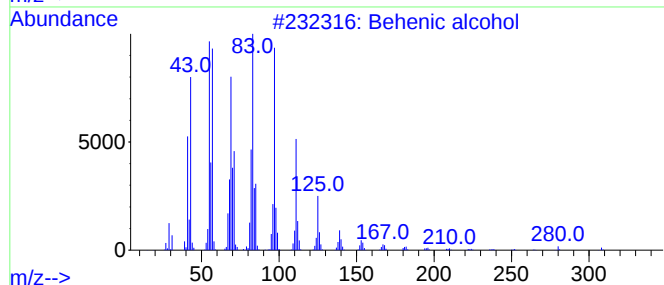
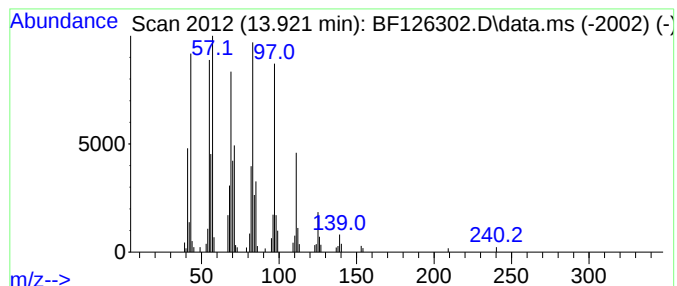
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Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	7.22 ng	596605	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Tricosene	322	C23H46	018835-32-0	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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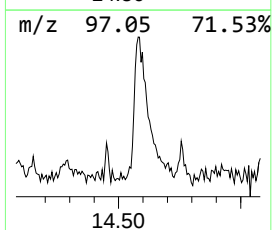
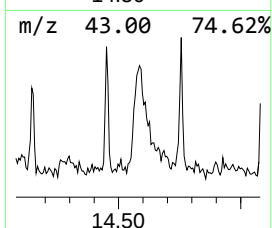
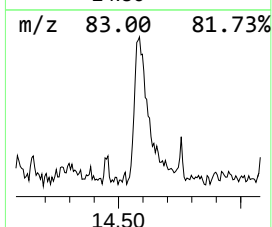
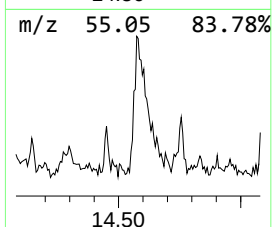
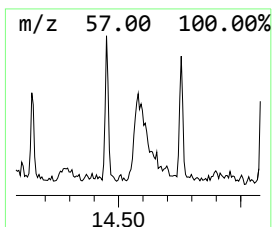
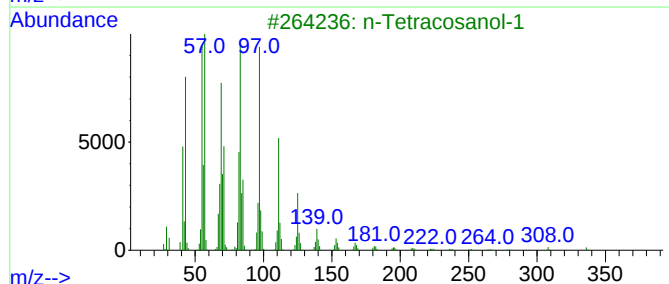
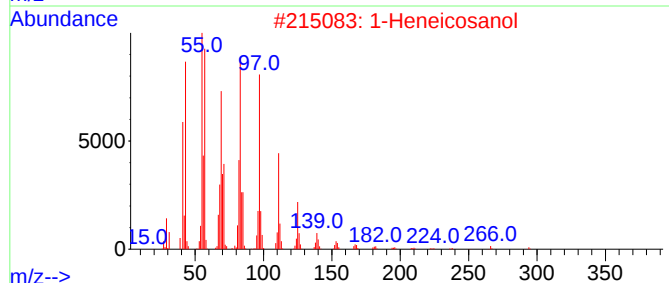
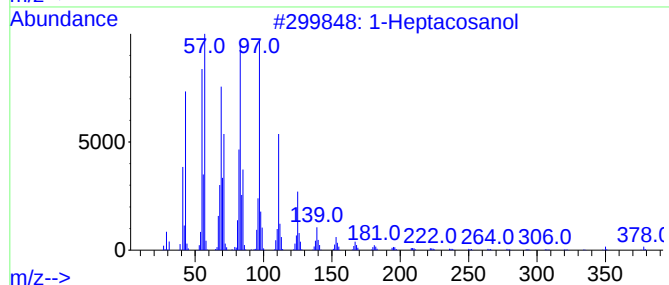
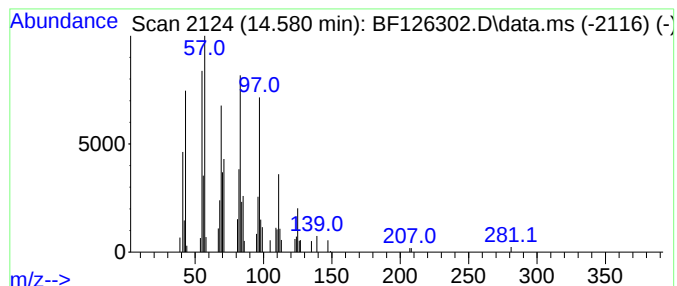
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Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	3.09 ng	255308	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			1-Hexacosene	364	C26H52	018835-33-1	93



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ClientSampleId :
TP9

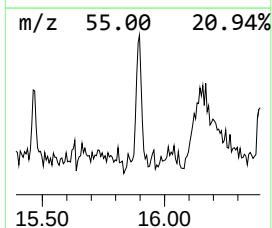
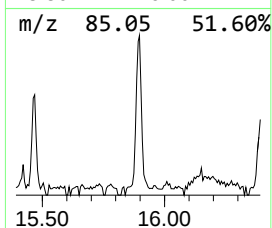
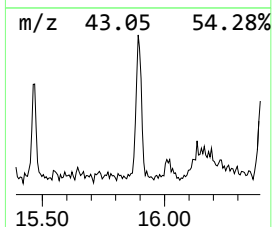
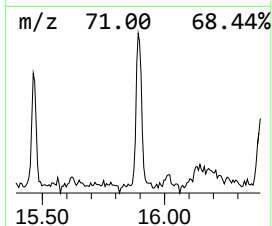
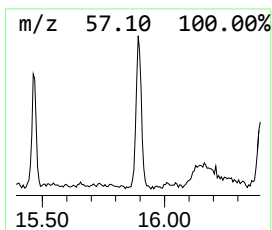
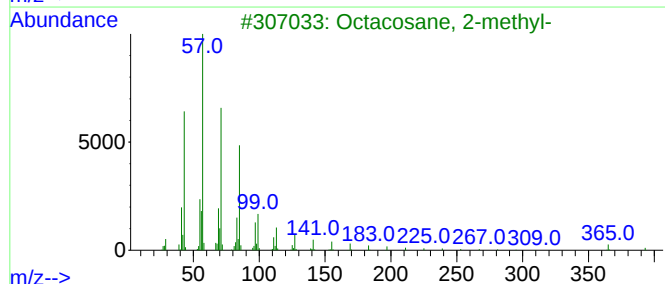
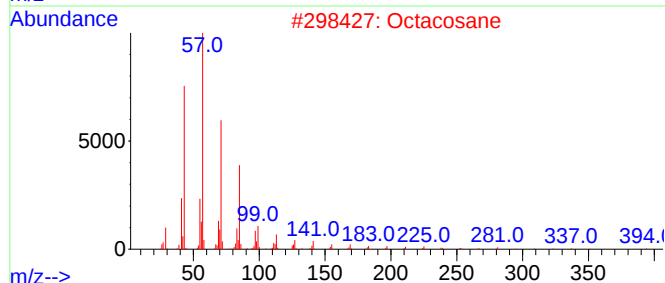
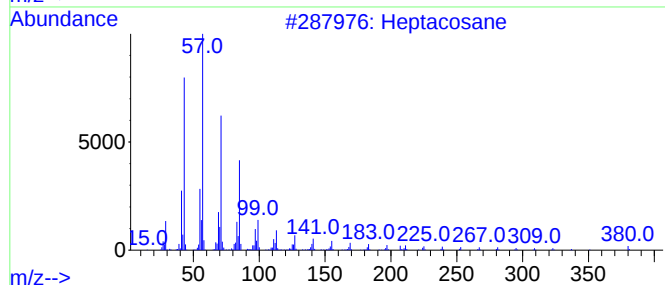
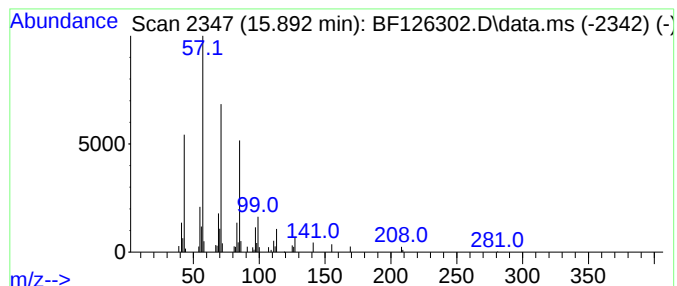
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.06 ng	108297	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
Data File : BF126302.D
Acq On : 21 Dec 2021 18:10
Operator : JU/CG
Sample : M5018-69
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	13.3	ng	808861	1	6.816	1219200	20.0
2-Pentanone, 4-...	5.034	14.2	ng	863767	1	6.816	1219200	20.0
Safrole	8.716	3.5	ng	308174	2	8.098	1742680	20.0
Behenic alcohol	13.921	7.2	ng	596605	5	13.974	1652610	20.0
1-Heptacosanol	14.580	3.1	ng	255308	5	13.974	1652610	20.0
Heptacosane	15.892	2.1	ng	108297	6	15.421	1050940	20.0