

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125217.D
 Acq On : 25 Aug 2021 19:14
 Operator : JU/CG
 Sample : M3467-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-10-(410.75)

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	16	22	28	rBV	985684	1220084	28.48%	3.069%
2	5.140	511	519	526	rBV	126696	158289	3.69%	0.398%
3	5.534	581	586	589	rBV	4628796	4284296	100.00%	10.777%
4	6.534	751	756	760	rBV	3874925	4216216	98.41%	10.605%
5	6.916	817	821	824	rBV	1626632	1315589	30.71%	3.309%
6	7.475	911	916	919	rBV	3236193	2742429	64.01%	6.898%
7	8.092	1018	1021	1035	rBV	358866	605855	14.14%	1.524%
8	8.198	1035	1039	1042	rBV	1899951	1647695	38.46%	4.145%
9	9.269	1217	1221	1224	rBV	4792418	3995403	93.26%	10.050%
10	9.951	1333	1337	1340	rBV	2013354	1709919	39.91%	4.301%
11	10.733	1467	1470	1474	rBV	2593209	2481831	57.93%	6.243%
12	11.433	1586	1589	1592	rBV	1578200	1545216	36.07%	3.887%
13	11.457	1592	1593	1597	rVV	408847	311356	7.27%	0.783%
14	11.510	1600	1602	1605	rVB	130075	100725	2.35%	0.253%
15	11.663	1622	1628	1634	rBV3	46482	64961	1.52%	0.163%
16	11.951	1669	1677	1682	rBV2	285409	405117	9.46%	1.019%
17	12.051	1690	1694	1696	rBV	103344	109904	2.57%	0.276%
18	12.486	1762	1768	1771	rBV2	54169	65420	1.53%	0.165%
19	12.569	1780	1782	1788	rVB2	51992	64092	1.50%	0.161%
20	12.651	1792	1796	1800	rVB	955233	820504	19.15%	2.064%
21	12.739	1808	1811	1814	rBV2	114658	101692	2.37%	0.256%
22	12.880	1829	1835	1838	rBV	795741	829290	19.36%	2.086%
23	12.927	1840	1843	1849	rVB3	52395	69363	1.62%	0.174%
24	13.022	1855	1859	1862	rBV	3332552	2875949	67.13%	7.234%
25	13.092	1867	1871	1875	rBV4	63051	104457	2.44%	0.263%
26	13.204	1888	1890	1893	rVB	112391	96685	2.26%	0.243%
27	13.274	1899	1902	1904	rVB	54272	48464	1.13%	0.122%
28	13.310	1904	1908	1911	rBV2	96561	100471	2.35%	0.253%
29	13.433	1926	1929	1933	rBV2	51677	63460	1.48%	0.160%
30	13.710	1973	1976	1981	rBV	107803	114870	2.68%	0.289%
31	13.827	1992	1996	1998	rVB2	72477	81416	1.90%	0.205%
32	13.857	1998	2001	2002	rBV	72108	57361	1.34%	0.144%
33	13.874	2002	2004	2008	rVB3	68584	72123	1.68%	0.181%
34	13.916	2008	2011	2013	rBV2	109802	98365	2.30%	0.247%
35	13.939	2013	2015	2018	rVV	77616	62162	1.45%	0.156%
36	14.074	2030	2038	2041	rBV2	1548704	1944177	45.38%	4.890%

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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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.104	2041	2043	2049	rVB	458341	439627	10.26%	1.106%
38	14.180	2054	2056	2059	rBV	60723	46705	1.09%	0.117%
39	14.463	2102	2104	2106	rVB	82283	60784	1.42%	0.153%
40	14.498	2107	2110	2114	rVB2	69823	66993	1.56%	0.169%
41	14.539	2114	2117	2123	rBV3	123484	163627	3.82%	0.412%
42	14.586	2123	2125	2128	rBV3	46654	57971	1.35%	0.146%
43	15.133	2213	2218	2221	rBV	471174	773218	18.05%	1.945%
44	15.204	2226	2230	2234	rVV2	309169	385274	8.99%	0.969%
45	15.239	2234	2236	2242	rVB	101219	118336	2.76%	0.298%
46	15.445	2267	2271	2277	rVB	285280	377771	8.82%	0.950%
47	15.504	2277	2281	2287	rVB	327050	390483	9.11%	0.982%
48	15.574	2288	2293	2297	rBV	1205464	1557913	36.36%	3.919%
49	16.051	2370	2374	2382	rVB	128998	205591	4.80%	0.517%
50	17.080	2543	2549	2556	rVB2	147226	303866	7.09%	0.764%
51	17.533	2622	2626	2636	rVB	110642	221820	5.18%	0.558%

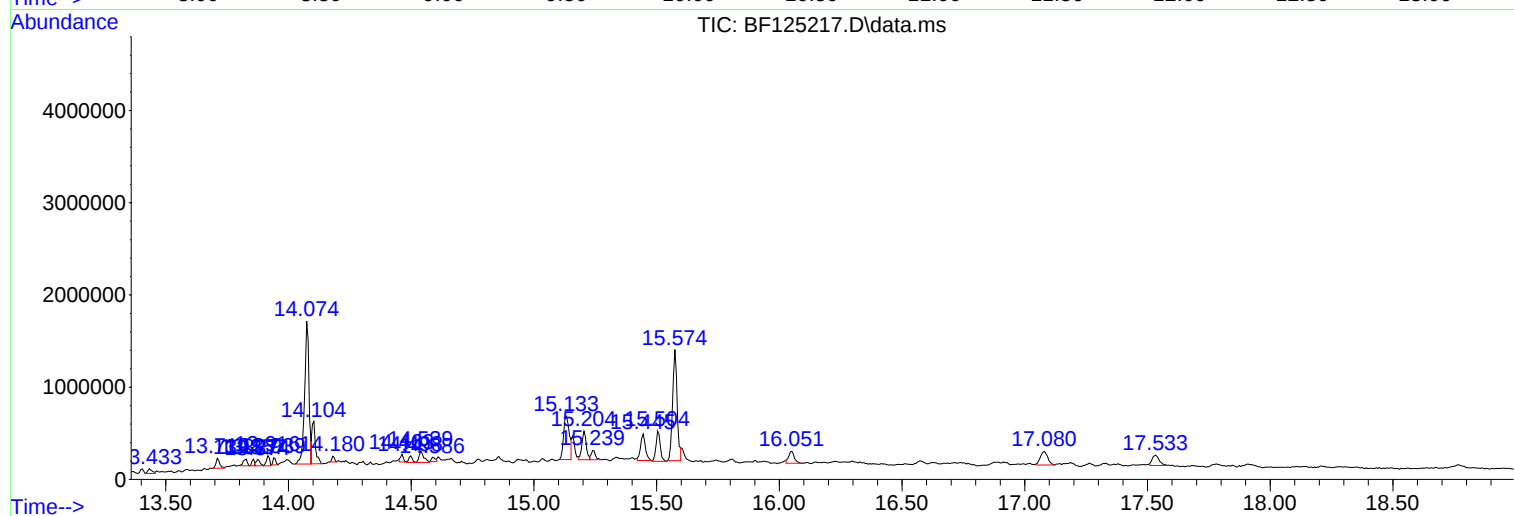
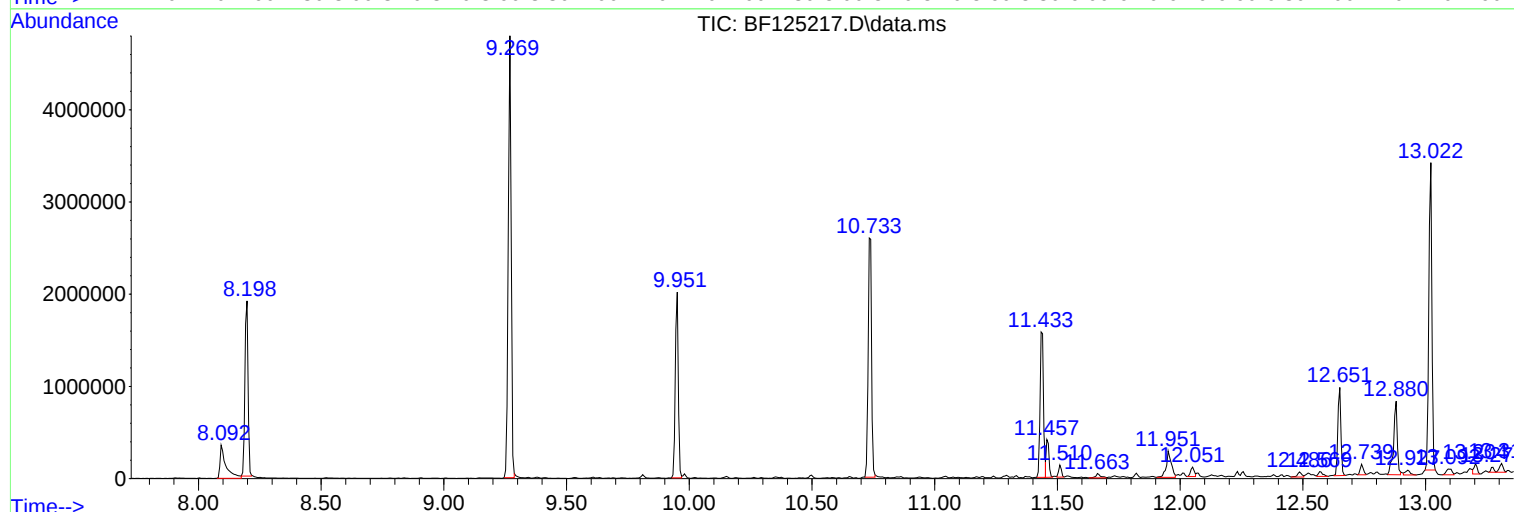
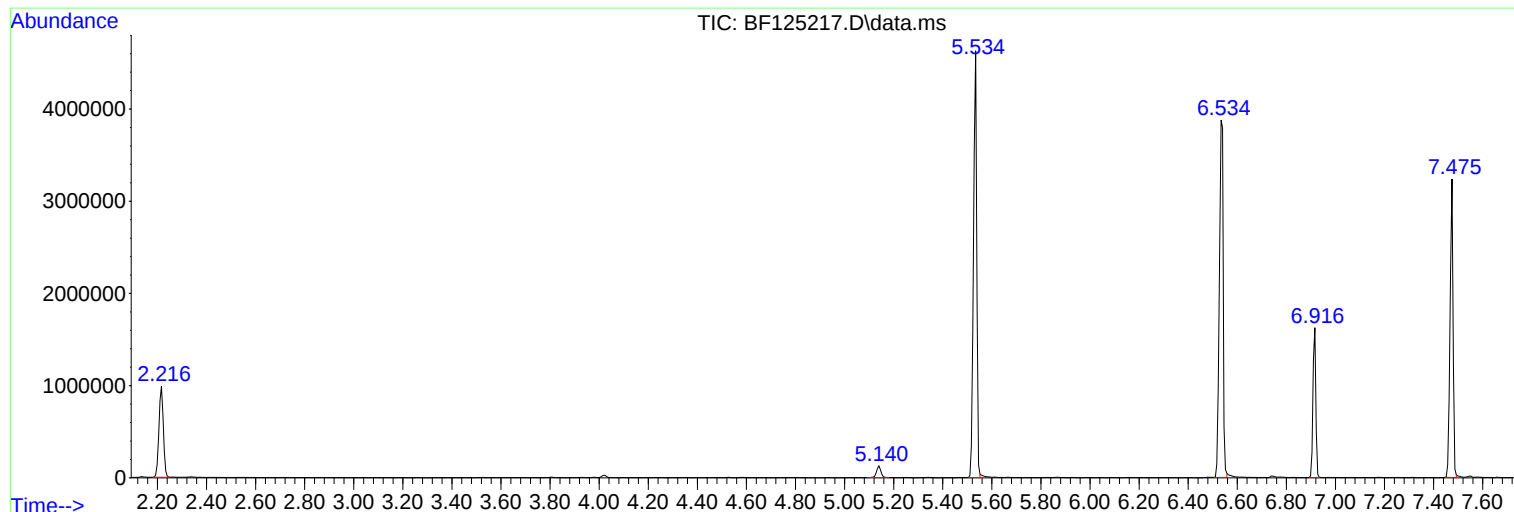
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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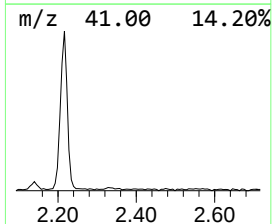
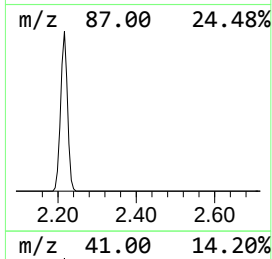
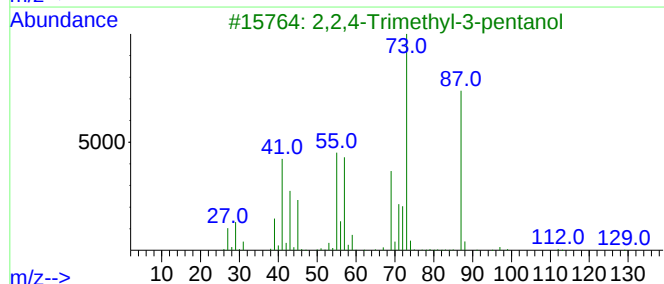
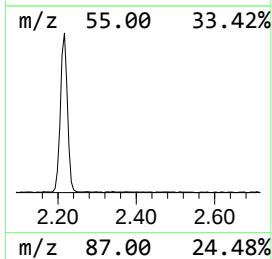
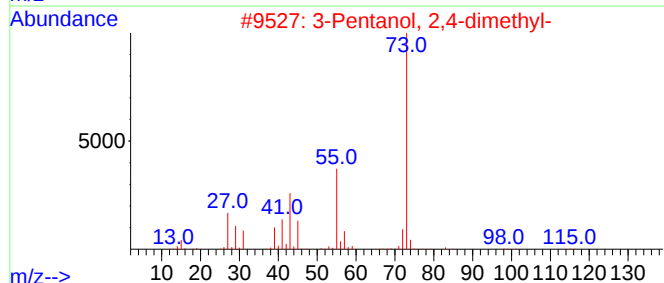
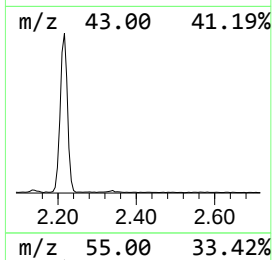
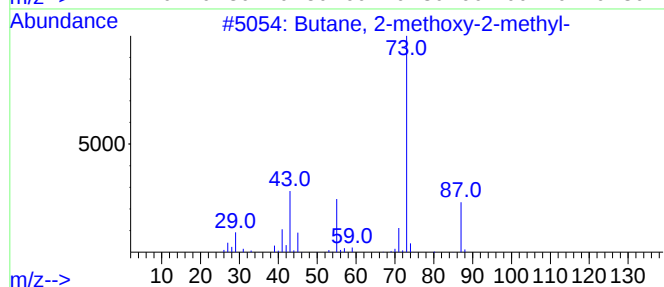
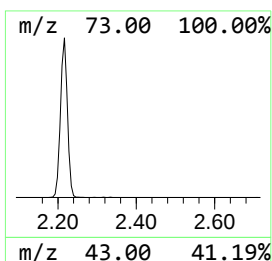
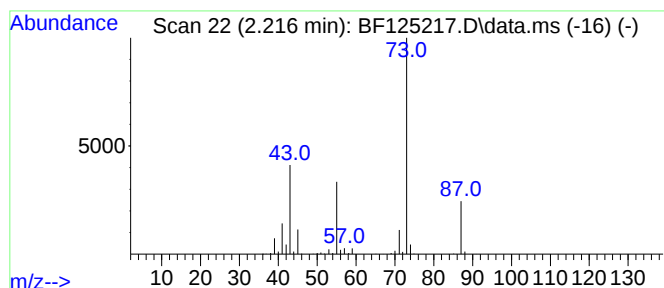
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	18.55 ng	1220080	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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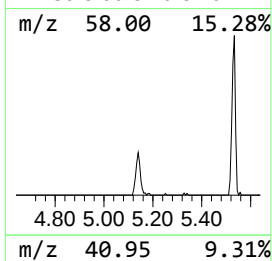
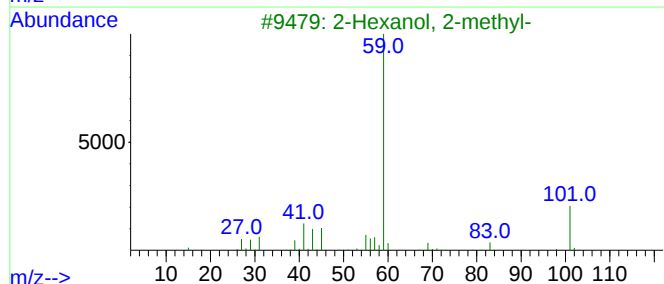
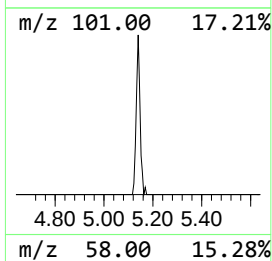
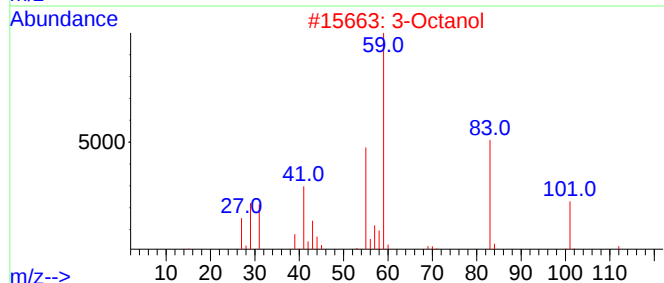
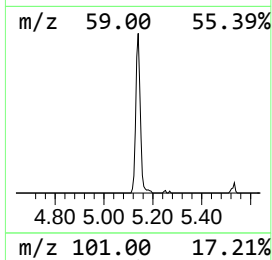
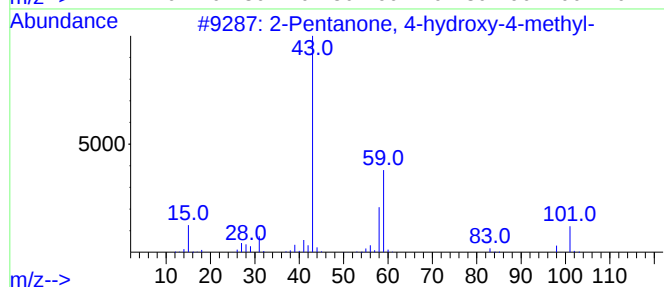
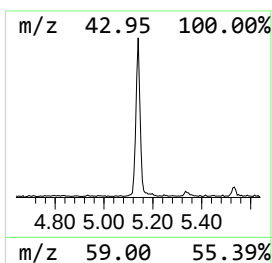
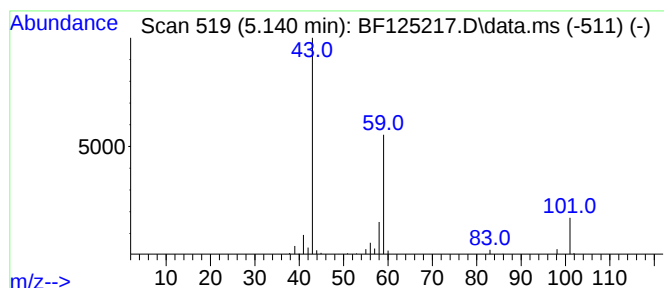
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.
5.140	2.41 ng	158289	1,4-Dichlorobenzene-d4		6.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	3-Octanol	130	C8H18O	000589-98-0	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	1,2-Butanediol	90	C4H10O2	000584-03-2	25	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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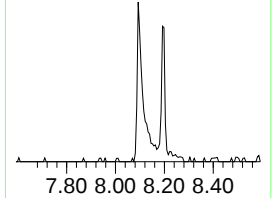
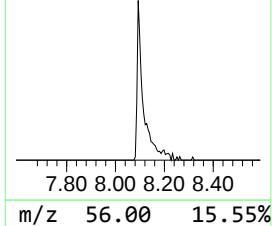
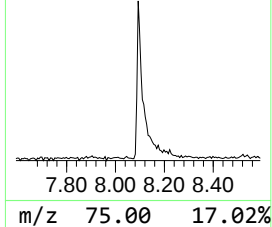
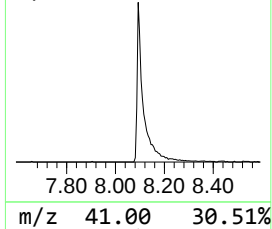
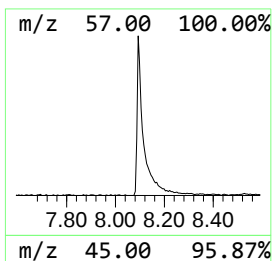
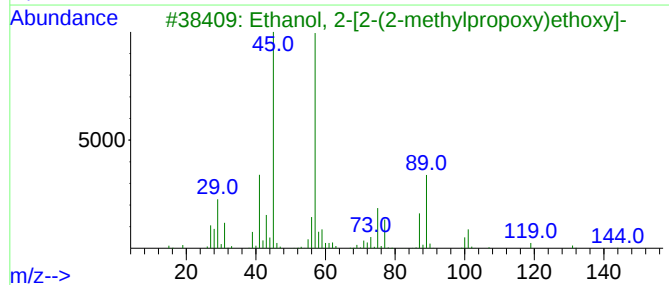
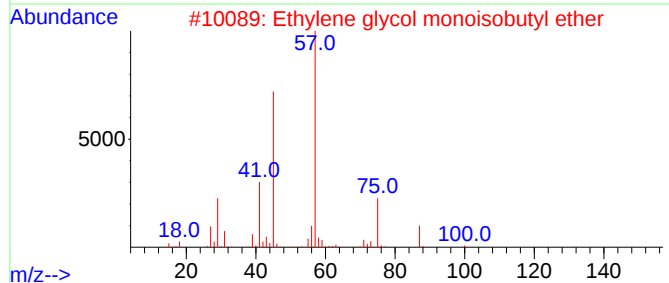
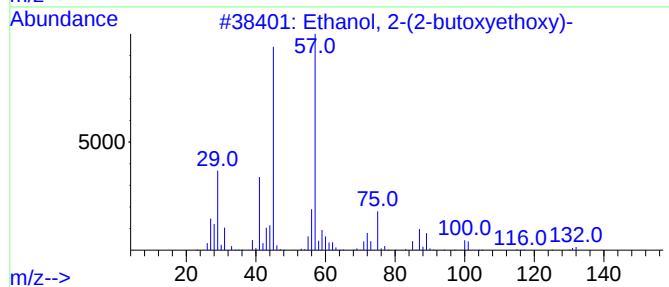
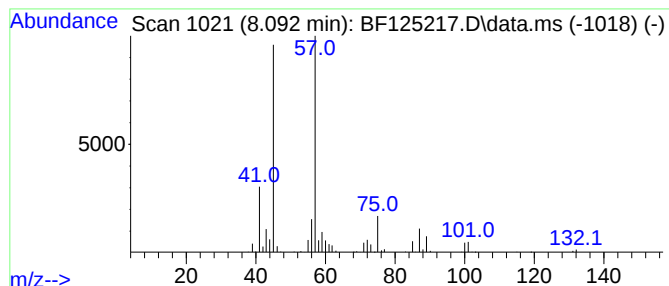
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	7.35 ng	605855	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5			Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	47



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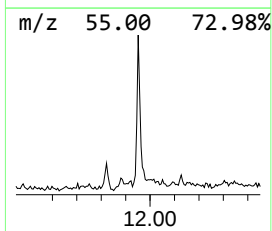
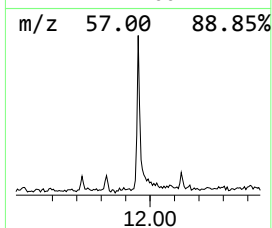
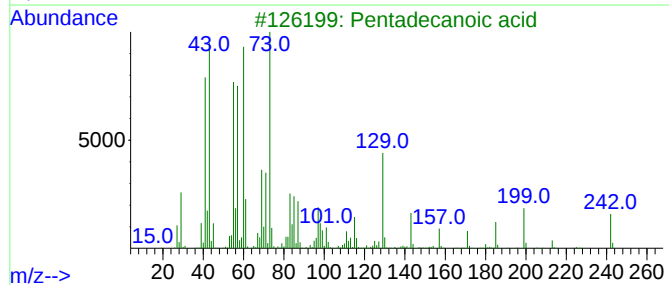
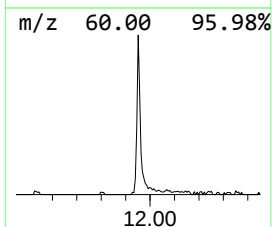
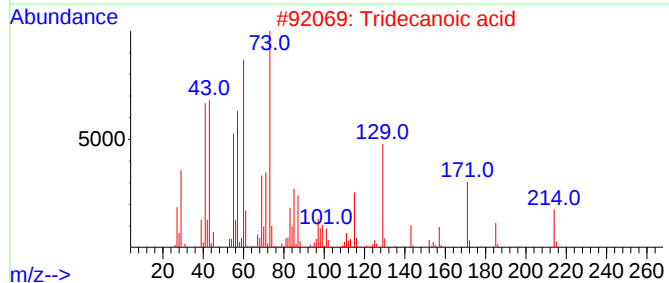
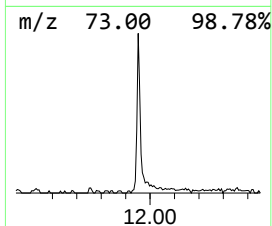
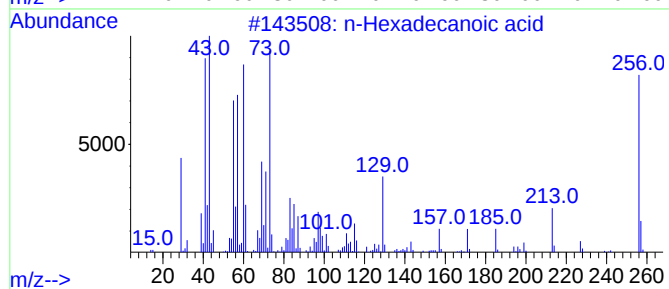
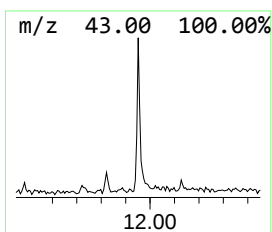
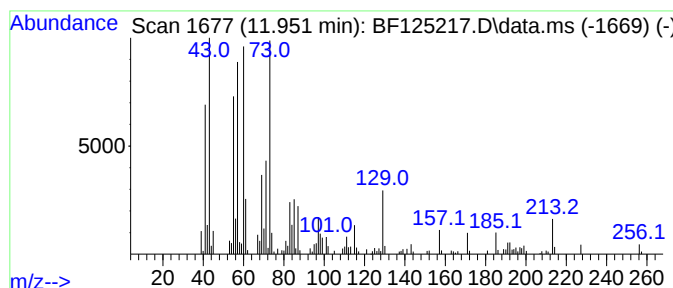
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.24 ng	405117	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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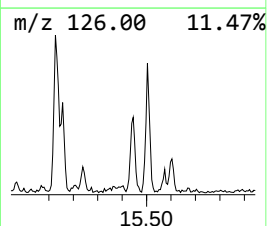
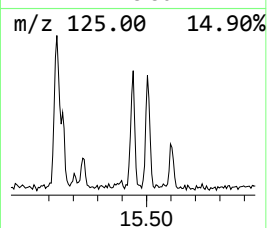
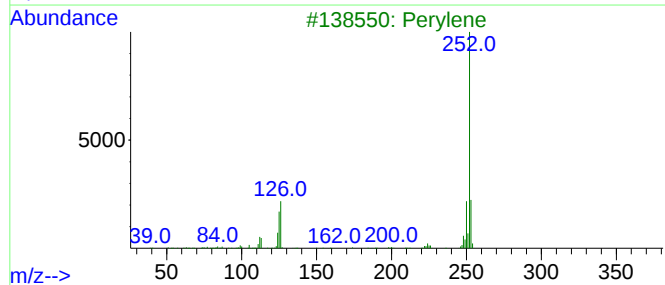
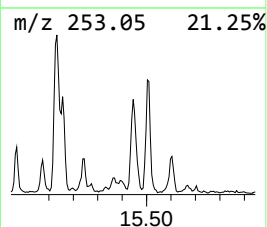
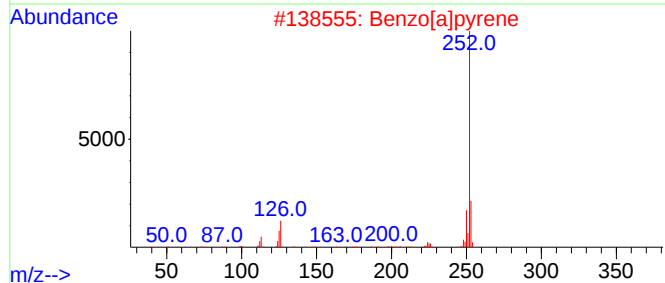
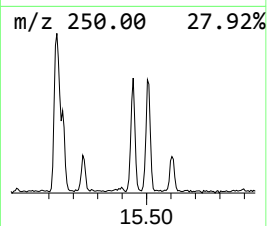
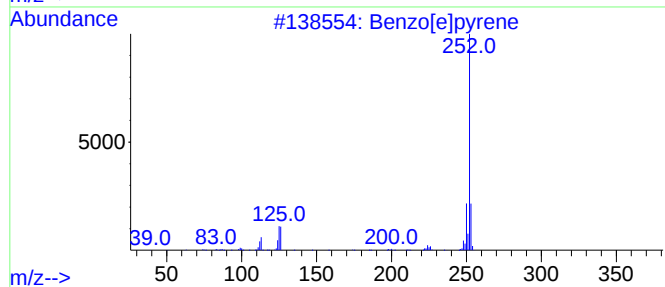
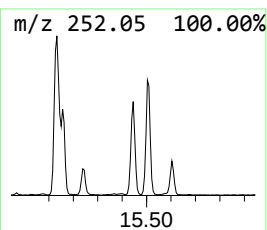
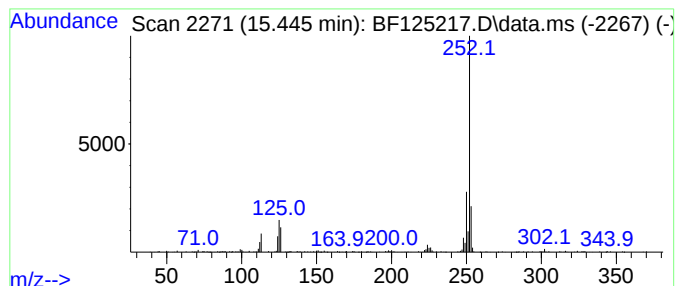
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	4.85 ng	377771	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Perylene	252	C20H12	000198-55-0	93
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125217.D
Acq On : 25 Aug 2021 19:14
Operator : JU/CG
Sample : M3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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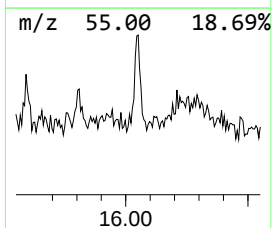
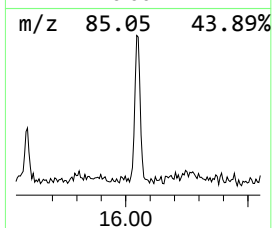
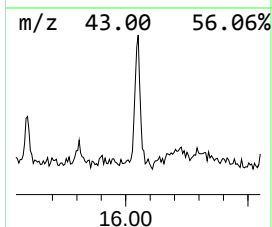
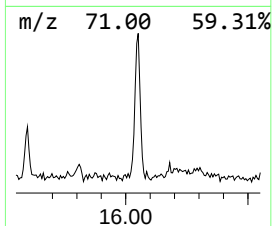
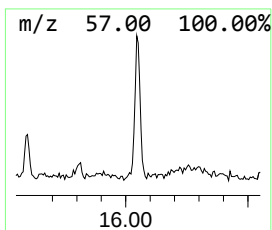
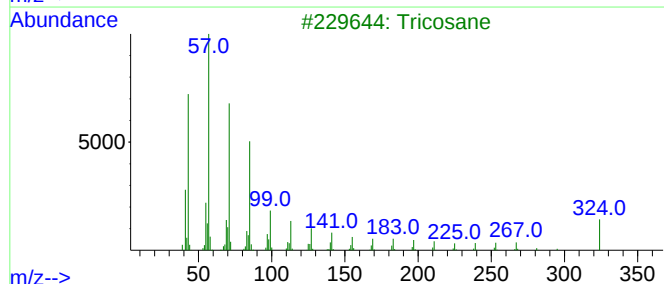
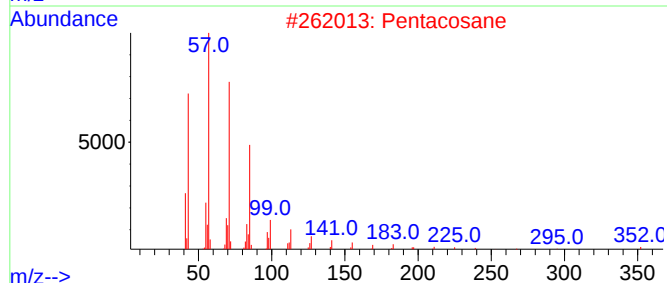
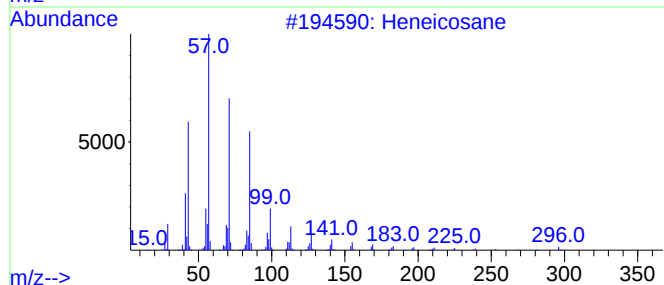
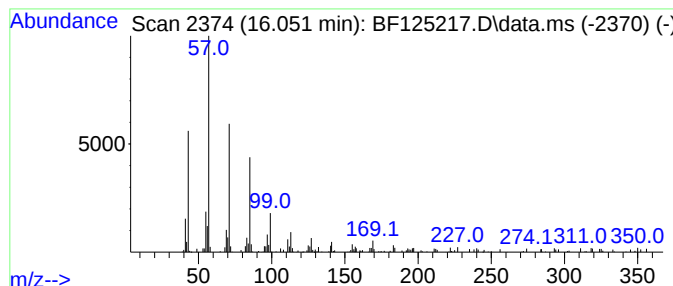
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	2.64 ng	205591	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Pentacosane	352	C25H52	000629-99-2	96
3			Tricosane	324	C23H48	000638-67-5	94
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125217.D
Acq On : 25 Aug 2021 19:14
Operator : JU/CG
Sample : M3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-10-(410.75)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	18.6	ng	1220080	1	6.916	1315590	20.0
2-Pentanone, 4-...	5.140	2.4	ng	158289	1	6.916	1315590	20.0
Ethanol, 2-(2-b...	8.092	7.3	ng	605855	2	8.198	1647700	20.0
n-Hexadecanoic ...	11.951	5.2	ng	405117	4	11.439	1545220	20.0
Benzo[e]pyrene	15.445	4.8	ng	377771	6	15.574	1557910	20.0
Heneicosane	16.051	2.6	ng	205591	6	15.574	1557910	20.0