

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041521\
 Data File : BF123576.D
 Acq On : 15 Apr 2021 19:51
 Operator : JU/CG
 Sample : M2007-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 55TH-ST-31

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-BF041521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	5498331	6997461	66.18%	11.517%
2	5.475	572	576	579	rBV	2107320	1788779	16.92%	2.944%
3	6.481	743	747	757	rBV	1301968	1189489	11.25%	1.958%
4	6.869	809	813	816	rVB	1925703	1660229	15.70%	2.733%
5	7.028	835	840	843	rBV	6026155	5332964	50.44%	8.778%
6	7.428	902	908	911	rBV	4526415	5069522	47.95%	8.344%
7	7.986	994	1003	1006	rBV	210450	389393	3.68%	0.641%
8	8.081	1012	1019	1023	rBV5	248929	617102	5.84%	1.016%
9	8.122	1023	1026	1028	rVV	331908	462052	4.37%	0.761%
10	8.151	1028	1031	1038	rVB	2771176	2426923	22.95%	3.995%
11	8.298	1051	1056	1061	rBV2	100768	126201	1.19%	0.208%
12	8.428	1074	1078	1085	rVB6	69203	118333	1.12%	0.195%
13	8.528	1085	1095	1099	rBV4	177757	398745	3.77%	0.656%
14	8.580	1099	1104	1106	rBV	104267	116046	1.10%	0.191%
15	9.233	1209	1215	1218	rBV	9388510	8418868	79.62%	13.857%
16	9.622	1278	1281	1285	rBV	274009	205803	1.95%	0.339%
17	9.910	1326	1330	1334	rVB	2560619	2345371	22.18%	3.860%
18	10.704	1459	1465	1468	rBV	4435699	4424138	41.84%	7.282%
19	11.404	1579	1584	1587	rBV	2915921	2498249	23.63%	4.112%
20	11.933	1670	1674	1685	rBV2	662029	806781	7.63%	1.328%
21	12.721	1805	1808	1816	rBV	190335	229407	2.17%	0.378%
22	13.004	1850	1856	1859	rBV	9749125	10573242	100.00%	17.403%
23	13.851	1995	2000	2003	rBV	88212	114344	1.08%	0.188%
24	13.886	2003	2006	2008	rVV	122378	129785	1.23%	0.214%
25	13.915	2008	2011	2017	rVB	302593	302980	2.87%	0.499%
26	14.051	2022	2034	2037	rBV	2460350	2542120	24.04%	4.184%
27	15.539	2281	2287	2291	rBV	1140552	1471861	13.92%	2.423%

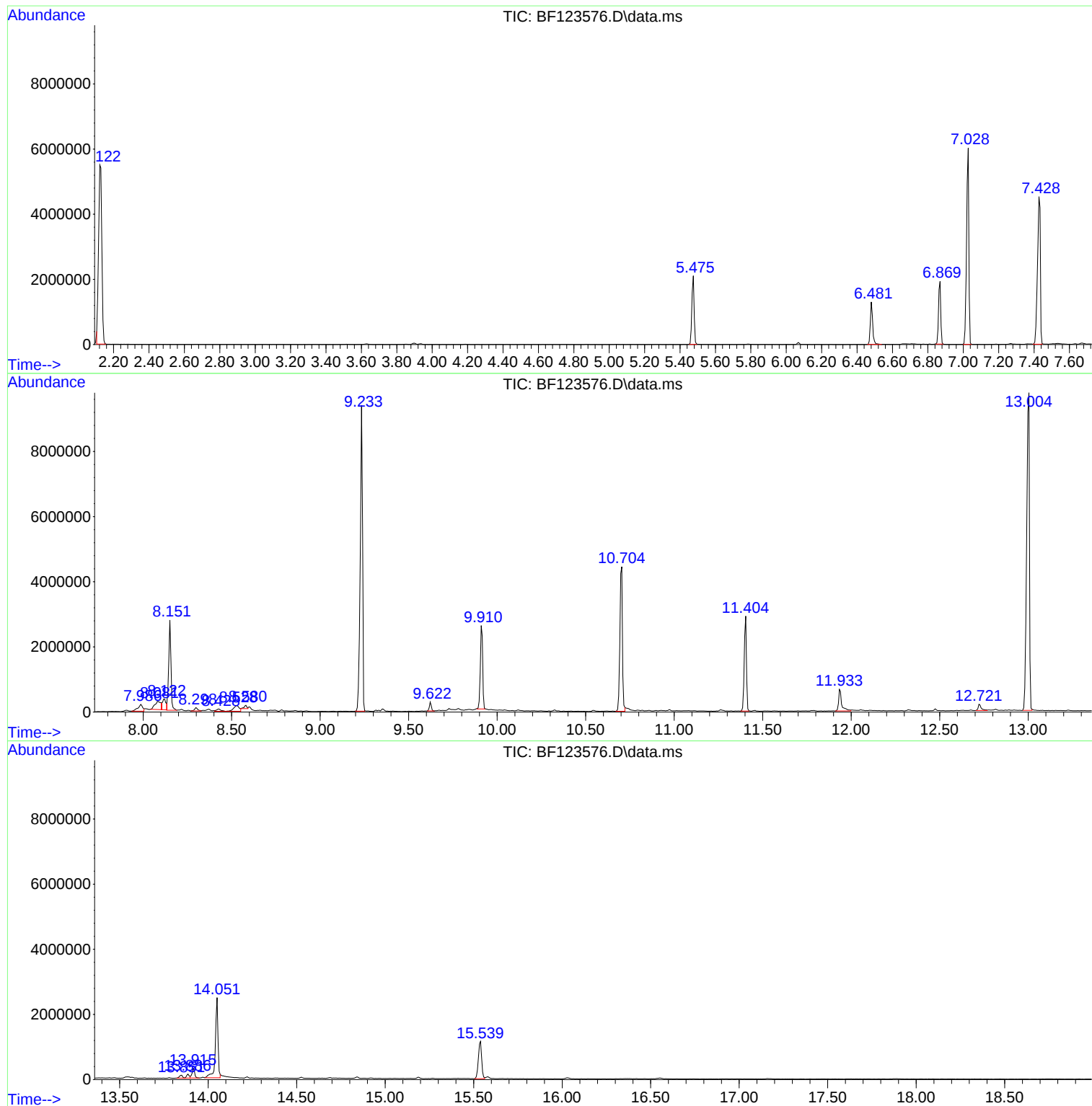
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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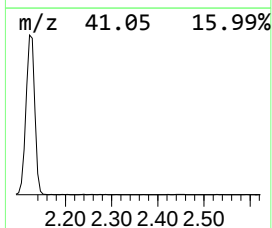
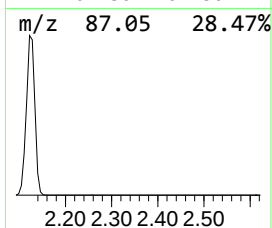
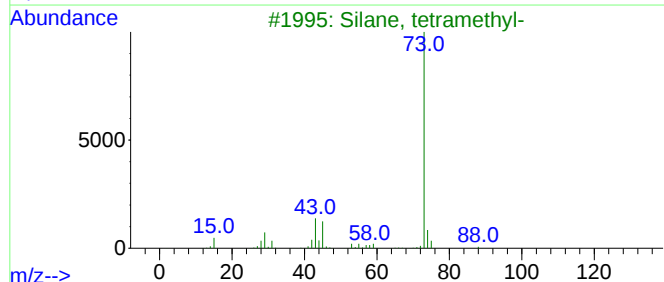
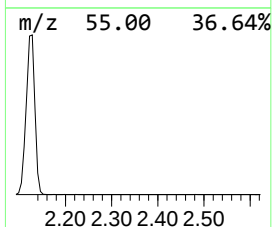
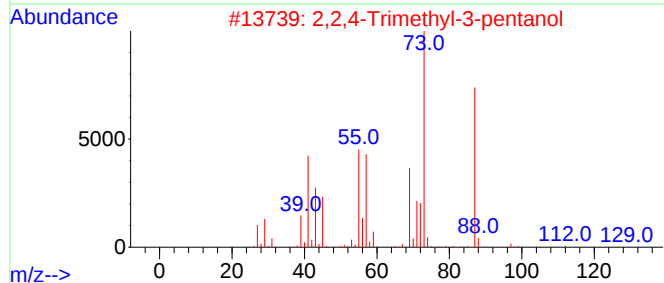
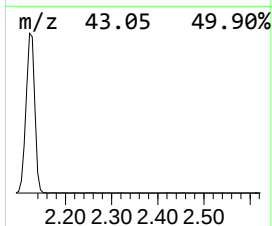
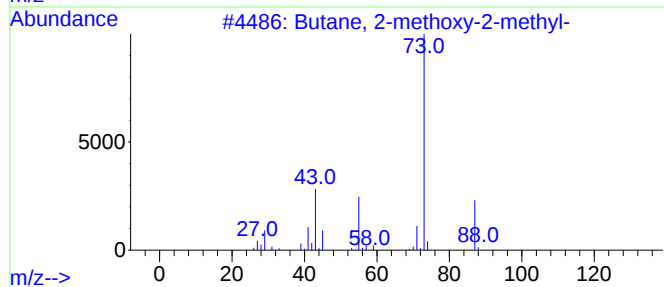
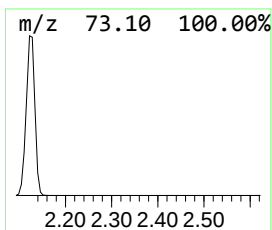
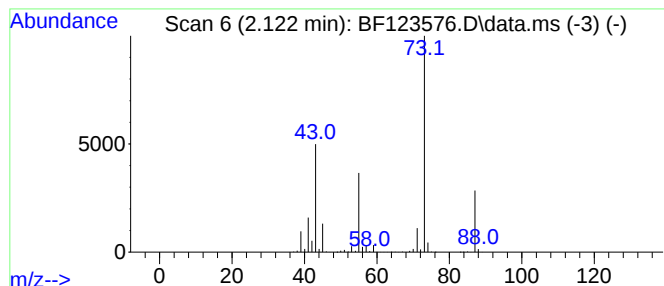
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.122	84.30 ng	6997460	1,4-Dichlorobenzene-d4	6.869

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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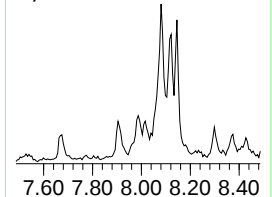
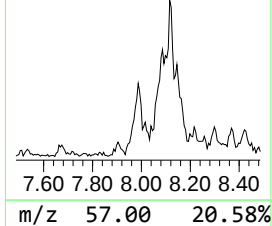
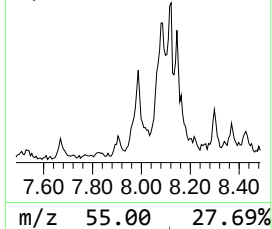
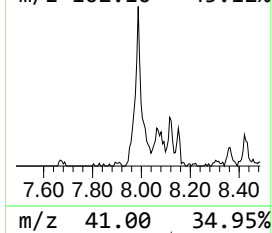
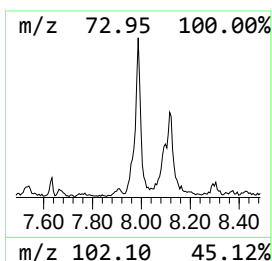
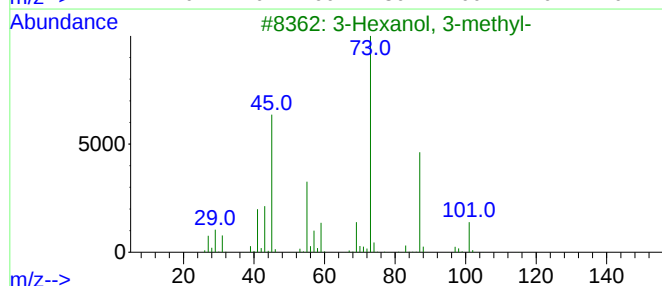
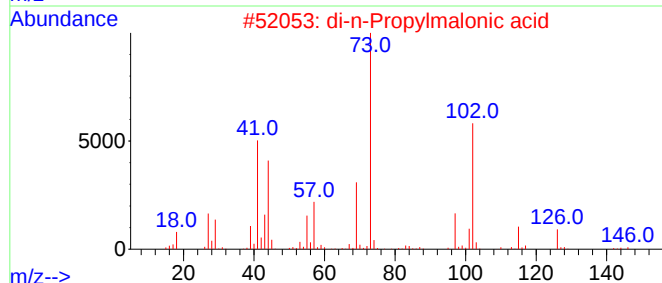
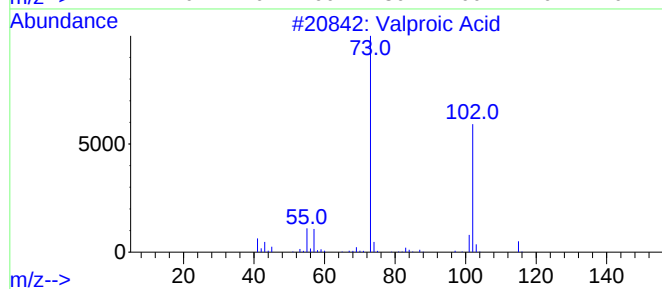
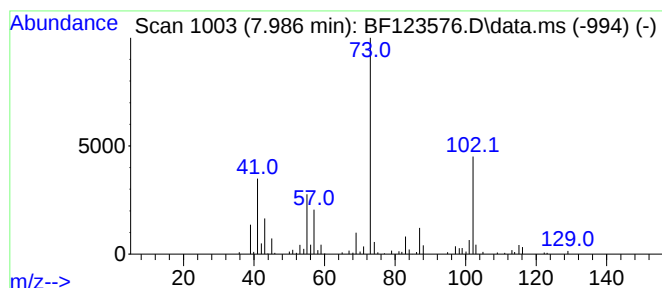
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Peak Number 3 Valproic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.986	3.21 ng	389393	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Valproic Acid	144	C8H16O2	000099-66-1	53
2			di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	40
3			3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	10
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	10
5			D-Mannotetradecane-1,2,3,4,5-pen...	278	C14H30O5	188436-16-0	10



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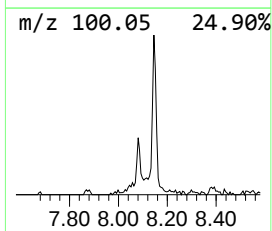
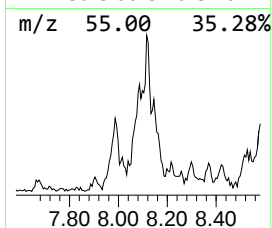
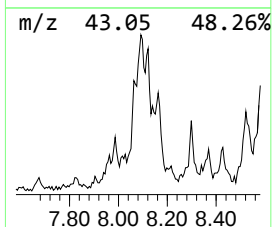
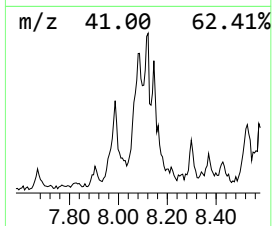
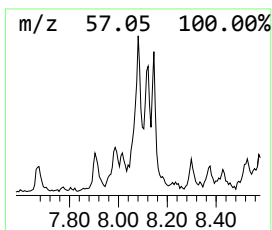
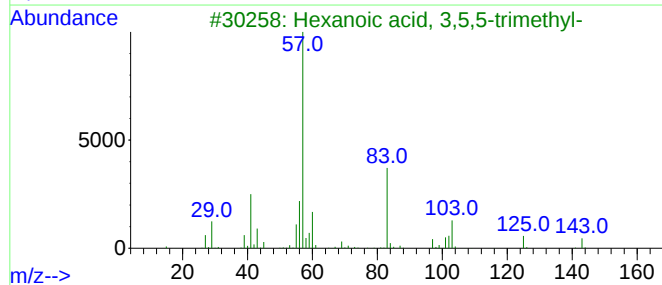
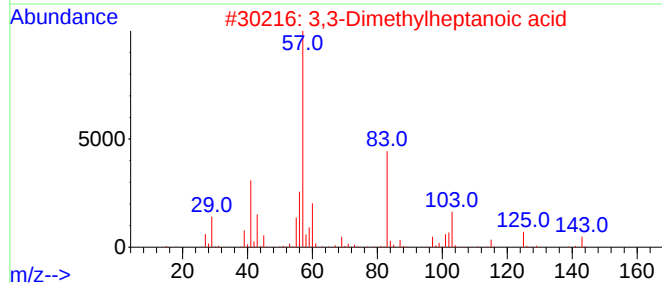
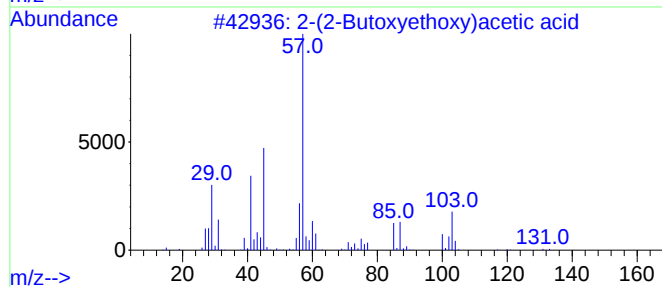
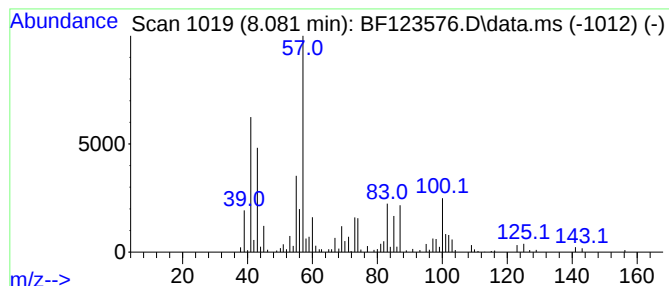
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.081 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	5.09 ng	617102	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)acetic acid		176	C8H16O4		082941-26-2	38
2	3,3-Dimethylheptanoic acid		158	C9H18O2		067061-30-7	37
3	Hexanoic acid, 3,5,5-trimethyl-		158	C9H18O2		003302-10-1	37
4	cis-1-Ethoxy-1-butene		100	C6H12O		1000139-43-8	25
5	2-Butanone, 3,3-dimethyl-		100	C6H12O		000075-97-8	22



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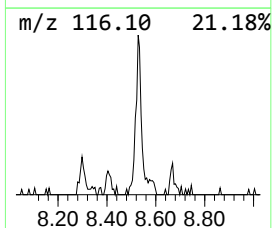
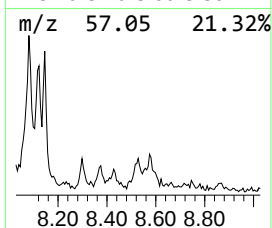
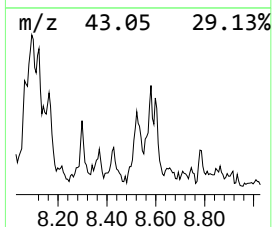
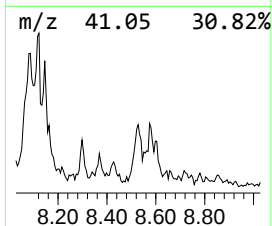
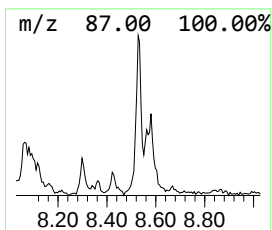
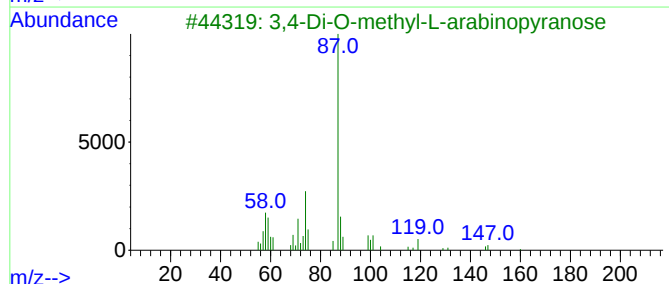
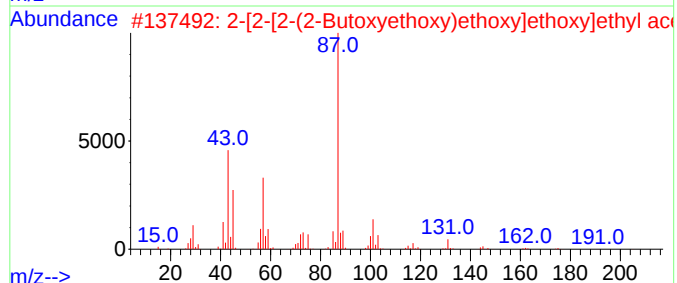
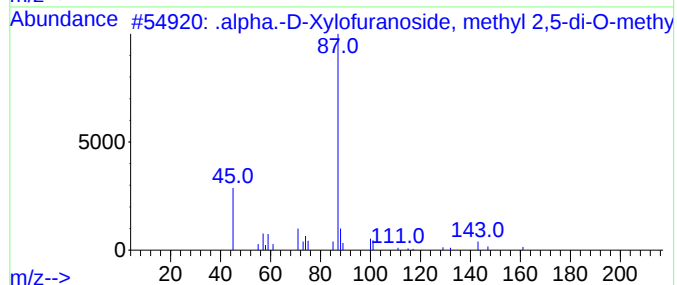
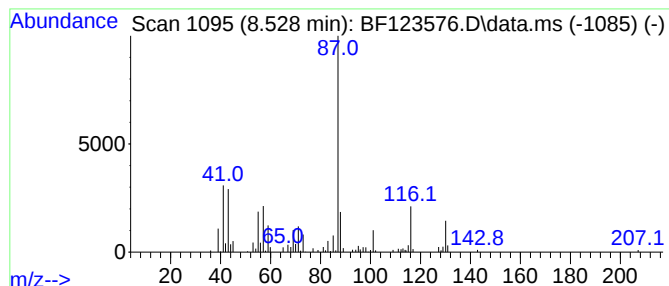
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Peak Number 5 .alpha.-D-Xylofuranoside, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.528	3.29 ng	398745	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	59
2	2-[2-[2-(2-Butoxyethoxy)ethoxy]e...	292	C14H28O6			1000351-93-9	50
3	3,4-Di-O-methyl-L-arabinopyranose	178	C7H14O5			086049-20-9	50
4	.alpha.-D-Xylofuranoside, methyl...	178	C7H14O5			032469-86-6	45
5	.alpha.-D-Xylofuranoside, methyl...	178	C7H14O5			034338-86-8	42



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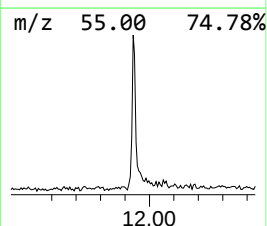
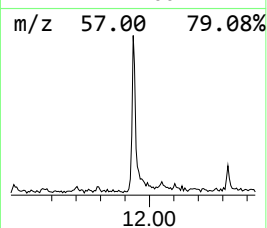
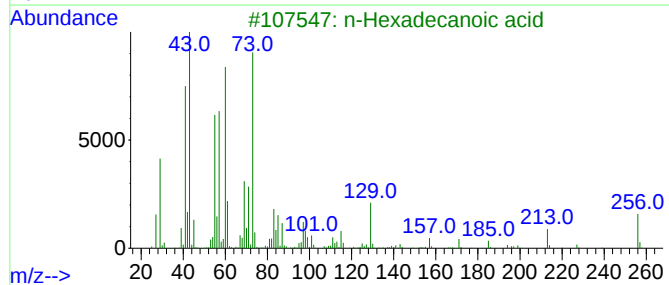
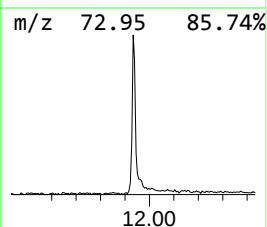
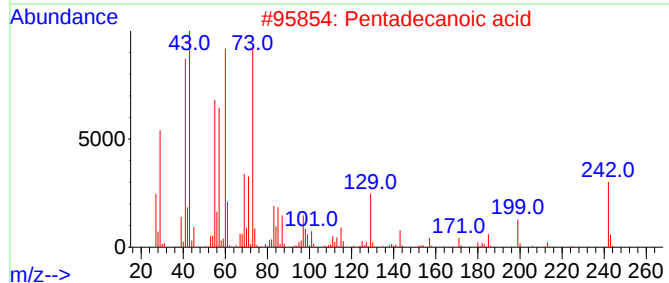
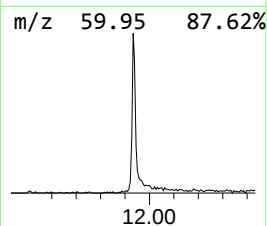
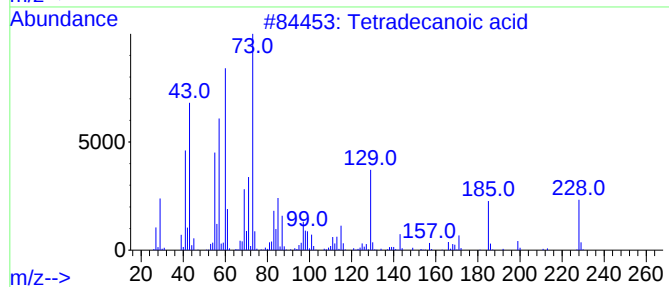
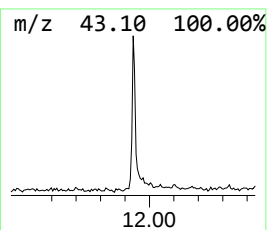
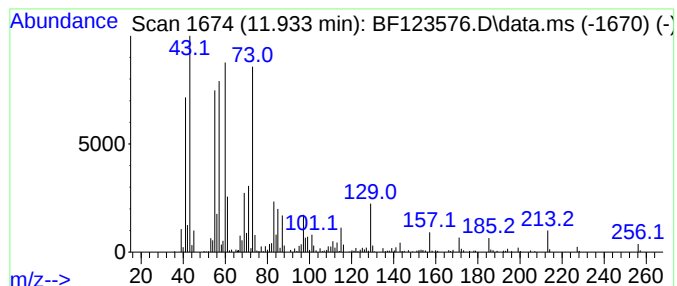
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.46 ng	806781	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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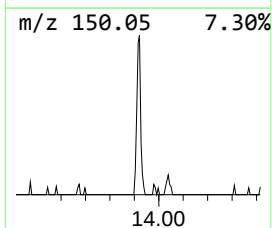
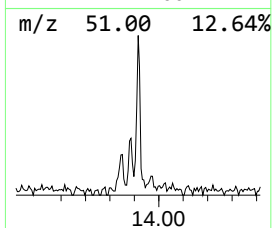
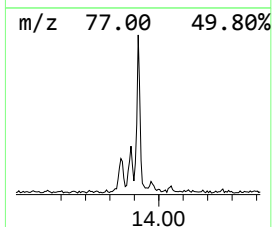
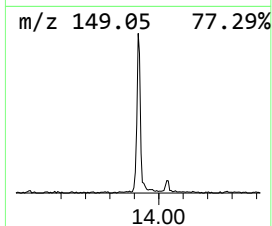
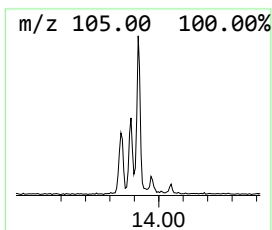
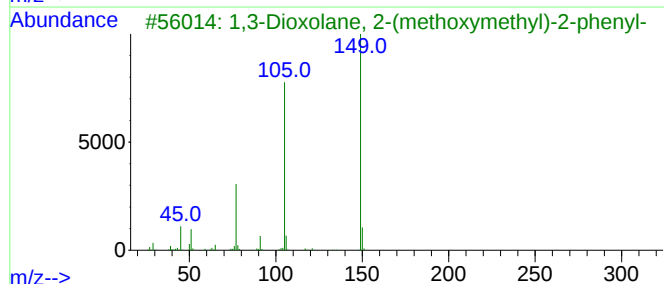
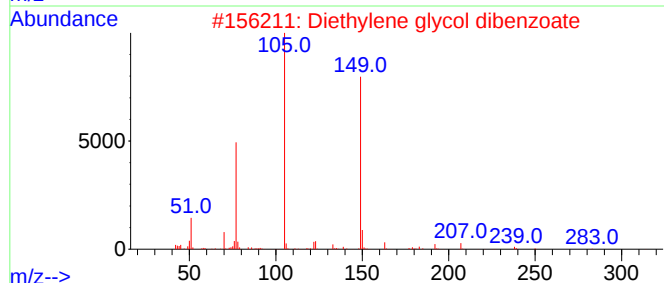
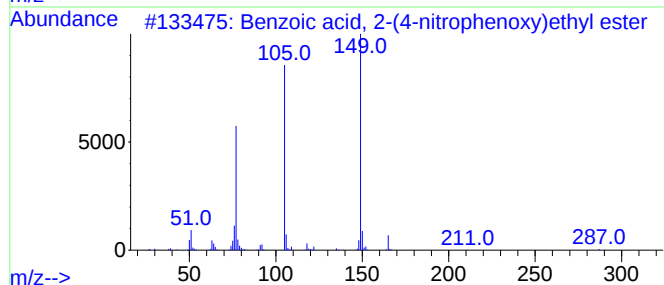
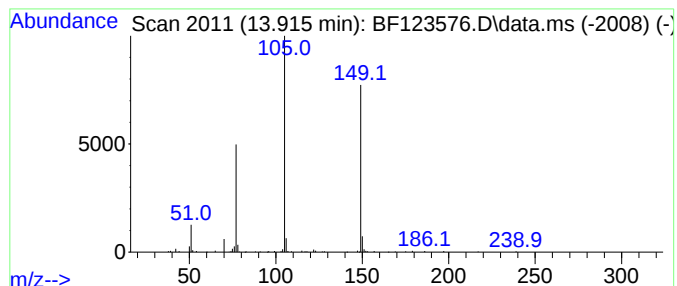
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2-(4-nitrophe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.38 ng	302980	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041521\
Data File : BF123576.D
Acq On : 15 Apr 2021 19:51
Operator : JU/CG
Sample : M2007-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
55TH-ST-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	84.3	ng	6997460	1	6.869	1660230	20.0
Valproic Acid	7.986	3.2	ng	389393	2	8.151	2426920	20.0
unknown8.081	8.081	5.1	ng	617102	2	8.151	2426920	20.0
.alpha.-D-Xylof...	8.528	3.3	ng	398745	2	8.151	2426920	20.0
Tetradecanoic acid	11.933	6.5	ng	806781	4	11.404	2498250	20.0
Benzoic acid, 2...	13.915	2.4	ng	302980	5	14.051	2542120	20.0