

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
 Data File : BM029325.D
 Acq On : 02 Apr 2021 17:47
 Operator : CG/JU
 Sample : M1874-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB16(26-27)

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_M\Methods\8270-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.946	5	10	14	rBV	424064	582903	11.70%	2.175%
2	2.987	14	17	23	rVB	92308	115124	2.31%	0.430%
3	4.846	328	333	341	rBV	56270	84991	1.71%	0.317%
4	5.298	403	410	418	rBV	1709163	2423377	48.65%	9.042%
5	6.875	666	678	689	rBV	1670705	2606925	52.34%	9.727%
6	7.698	812	818	825	rBV	413423	648376	13.02%	2.419%
7	8.851	1004	1014	1027	rBV	1011948	1658759	33.30%	6.189%
8	10.480	1284	1291	1299	rBV	509278	829869	16.66%	3.096%
9	12.957	1703	1712	1724	rBV	2298946	3367334	67.60%	12.564%
10	13.792	1848	1854	1864	rBV	90317	136611	2.74%	0.510%
11	14.163	1913	1917	1928	rVB3	22882	55054	1.11%	0.205%
12	14.333	1939	1946	1958	rVB	715599	1034564	20.77%	3.860%
13	15.821	2192	2199	2212	rBV	1621116	2402363	48.23%	8.963%
14	17.068	2405	2411	2422	rBV	817270	1175697	23.60%	4.387%
15	17.974	2560	2565	2574	rBV	92333	160301	3.22%	0.598%
16	19.250	2778	2782	2791	rBV4	43118	77931	1.56%	0.291%
17	19.697	2852	2858	2864	rBV	4361470	4981161	100.00%	18.585%
18	20.968	3070	3074	3084	rBV	475653	657811	13.21%	2.454%
19	21.244	3116	3121	3126	rBV	1122242	1371513	27.53%	5.117%
20	22.286	3294	3298	3306	rBV	692726	976499	19.60%	3.643%
21	23.456	3491	3497	3507	rVB2	777720	1454809	29.21%	5.428%

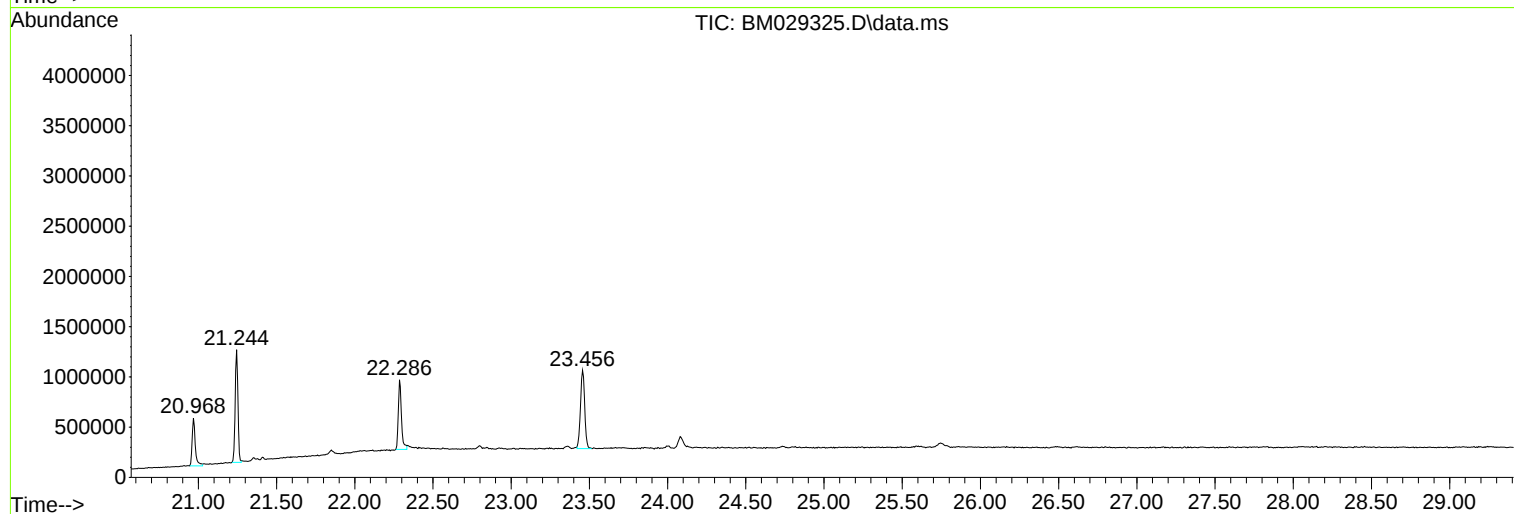
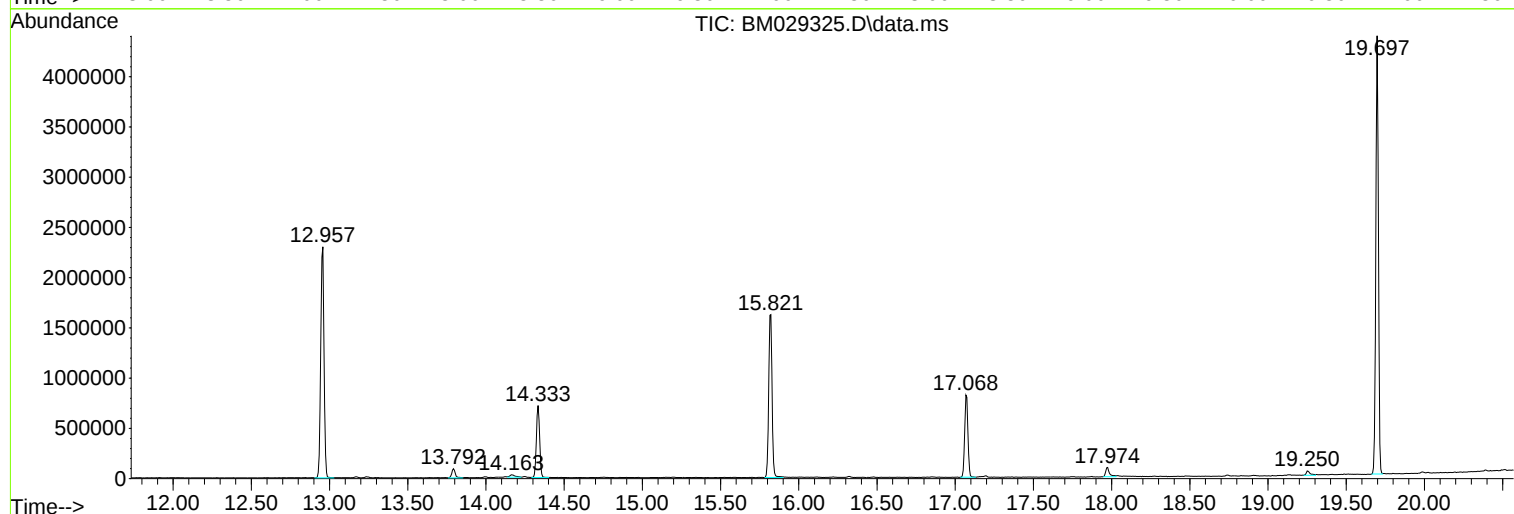
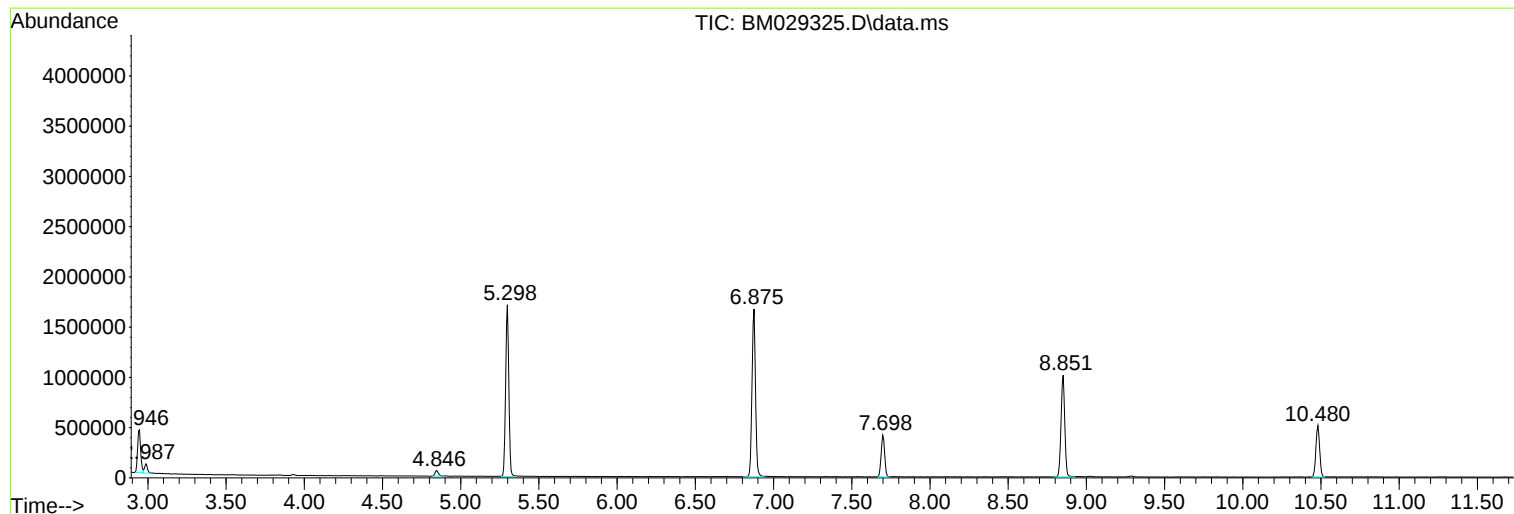
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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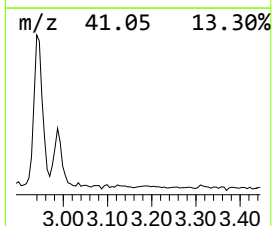
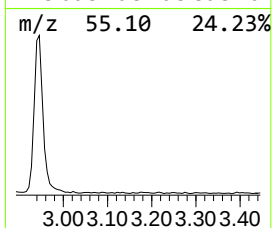
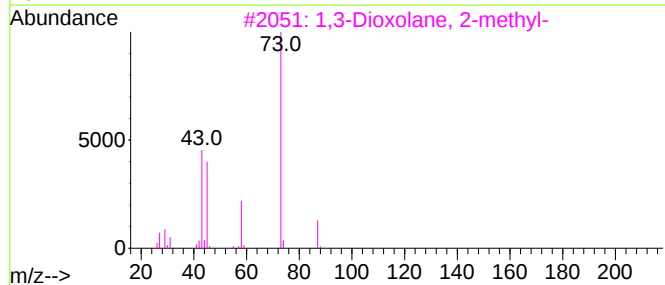
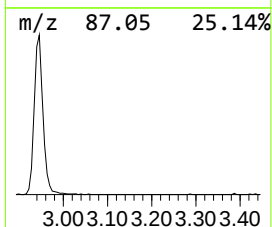
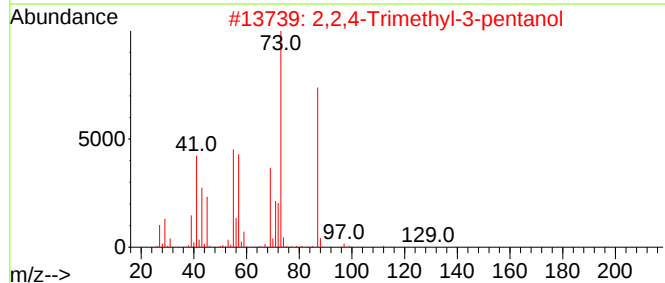
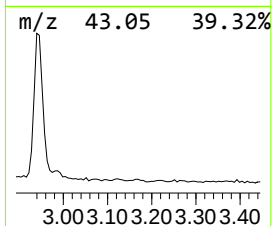
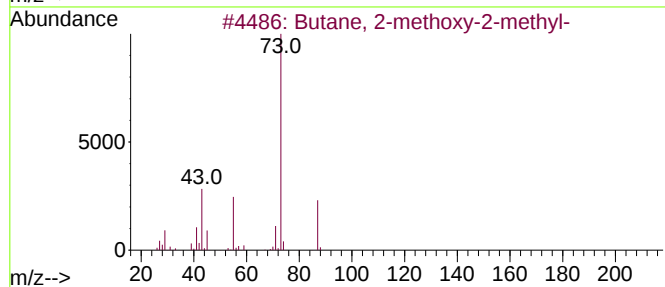
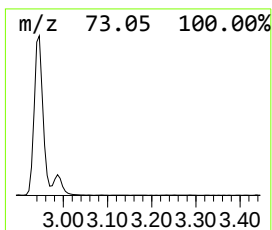
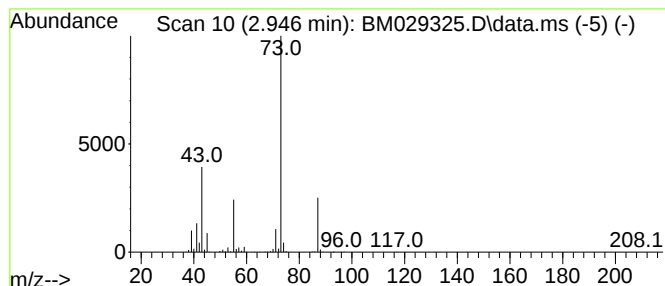
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.946	17.98 ng	582903	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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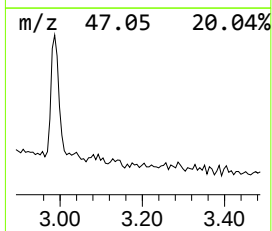
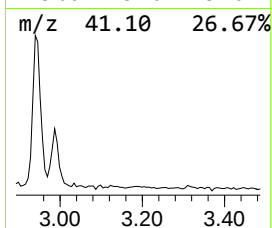
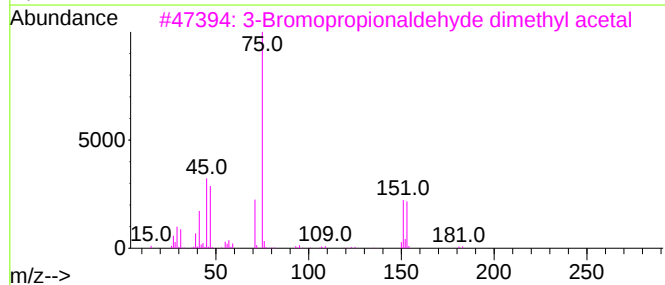
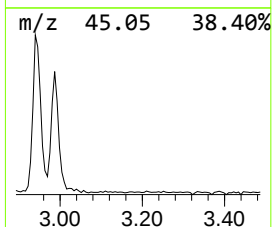
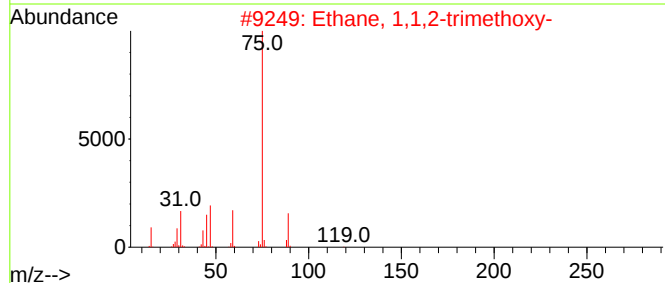
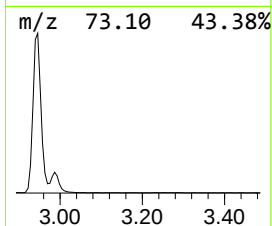
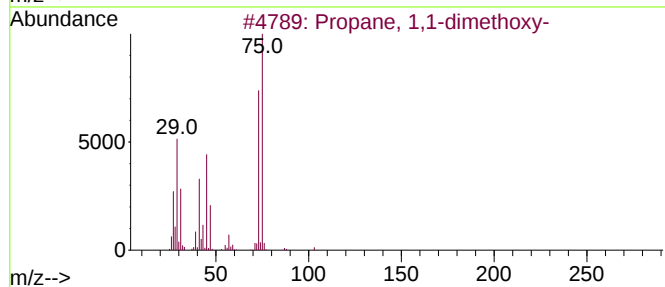
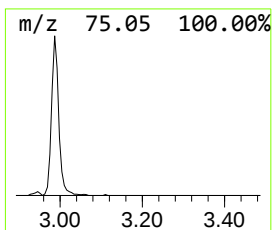
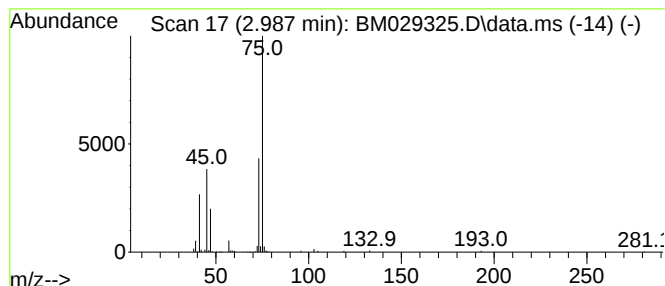
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Peak Number 2 unknown2.987 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.987	3.55 ng	115124	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	43
2			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9
3			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	9
4			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5			Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	9



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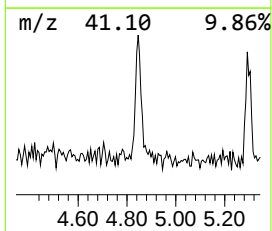
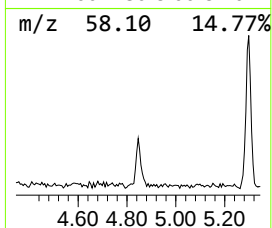
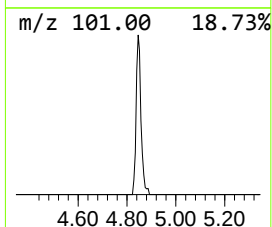
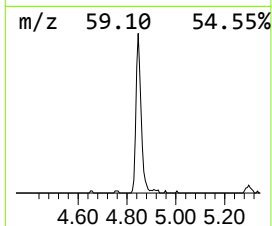
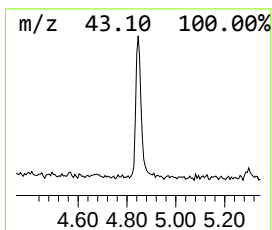
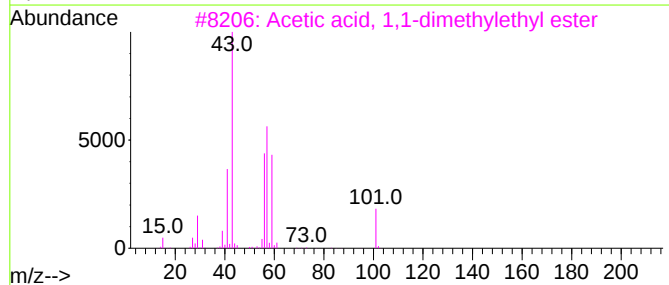
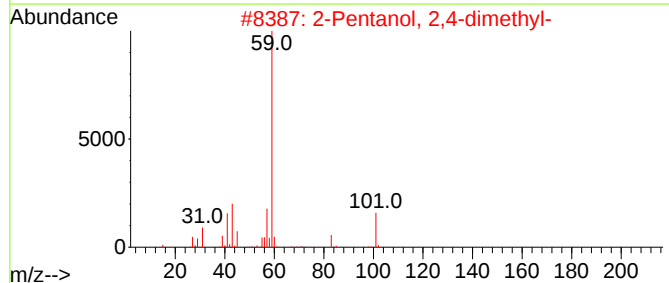
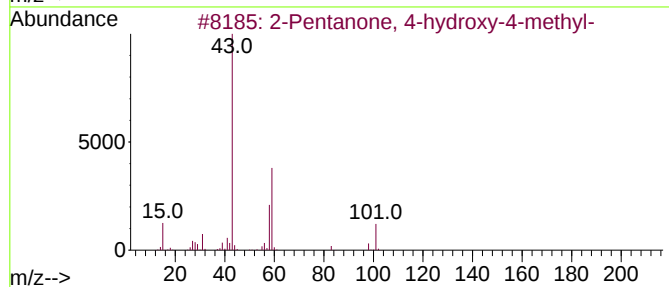
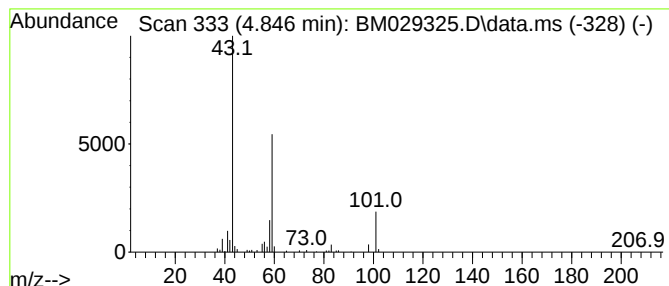
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.846	2.62 ng	84991	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	47		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	30		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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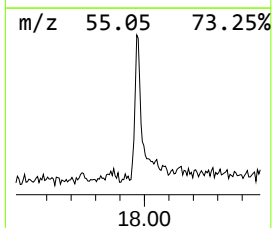
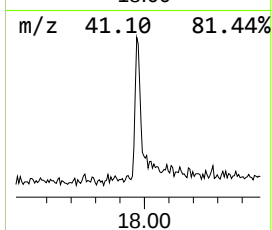
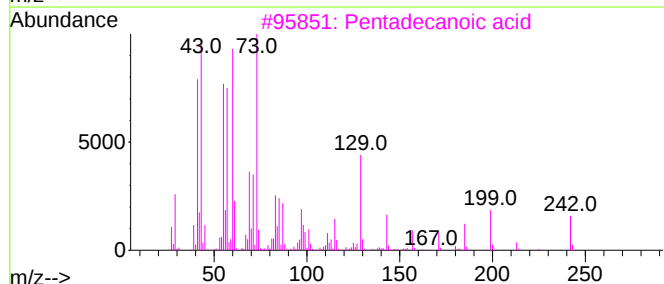
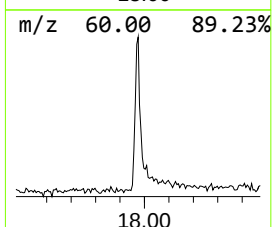
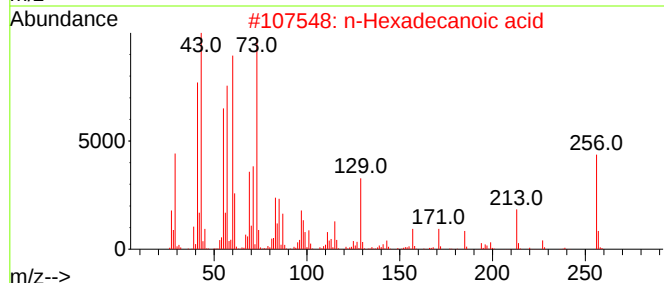
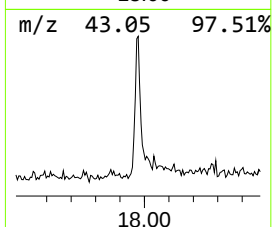
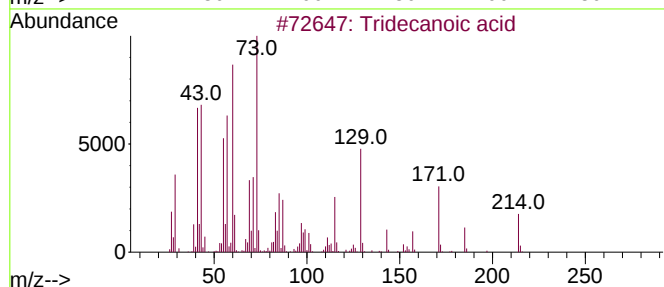
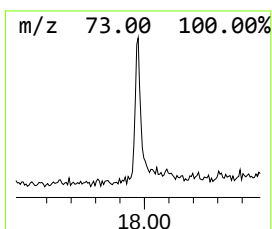
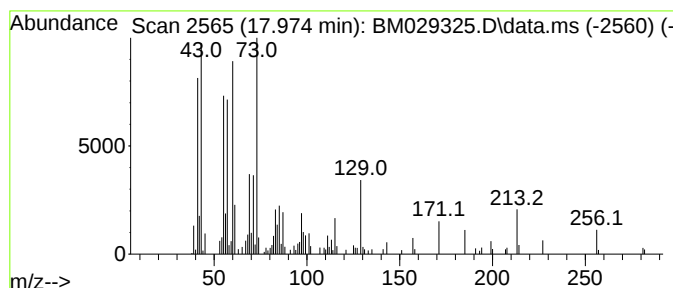
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	2.73 ng	160301	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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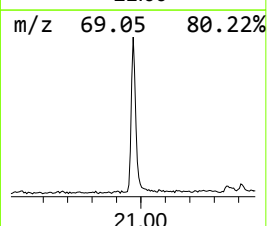
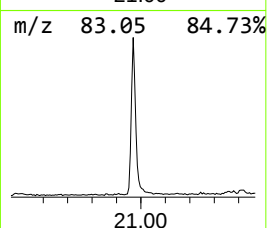
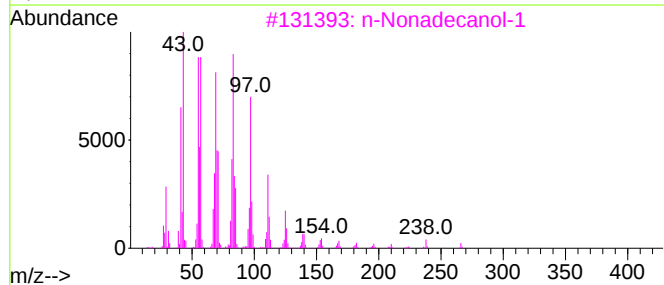
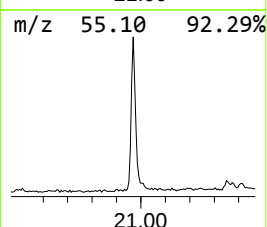
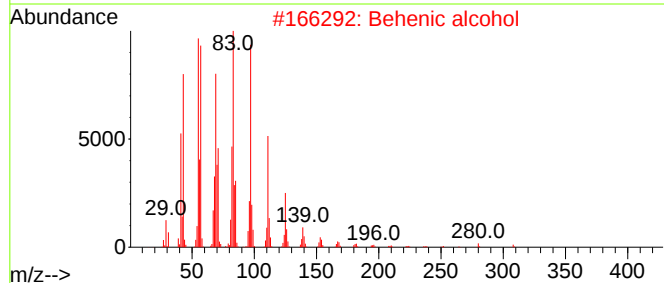
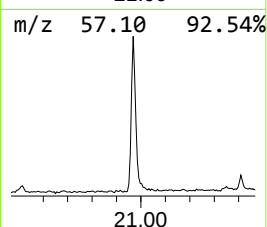
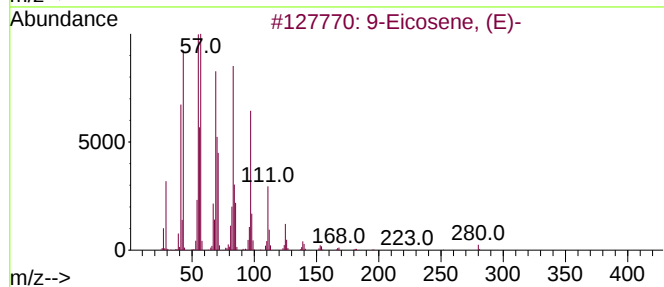
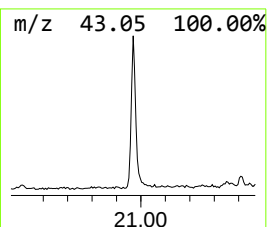
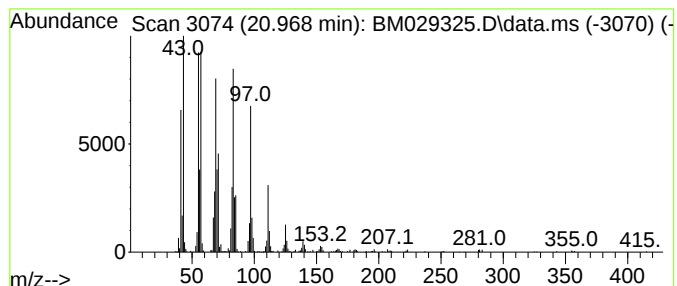
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Peak Number 5 9-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	9.59 ng	657811	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Eicosene, (E)-	280	C20H40	074685-29-3	96
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



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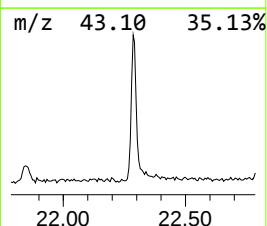
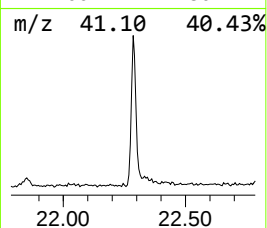
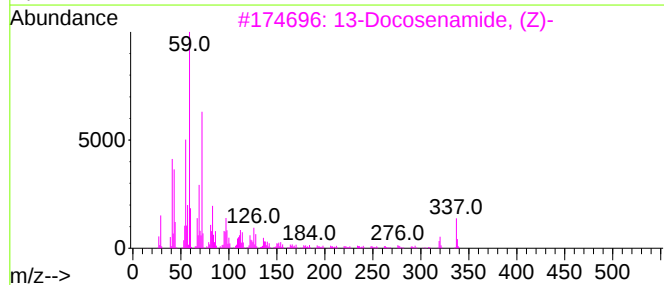
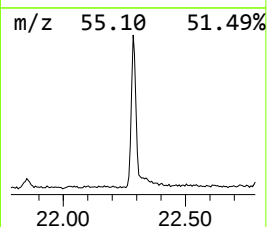
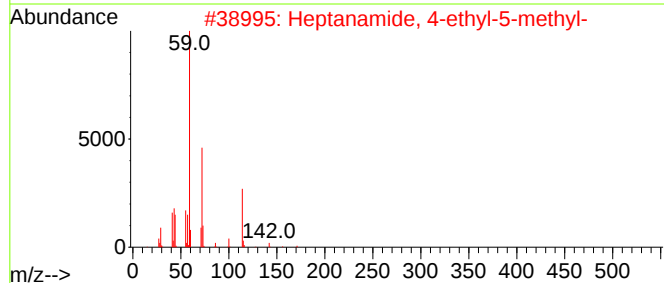
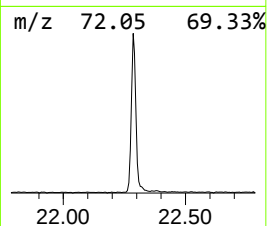
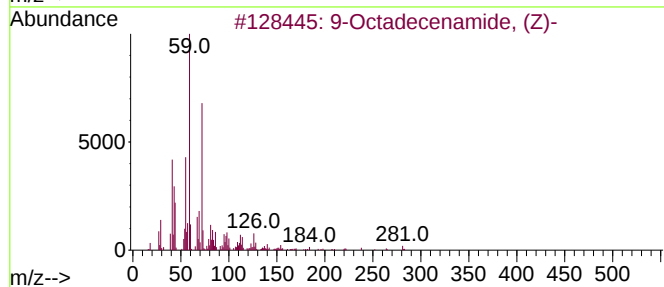
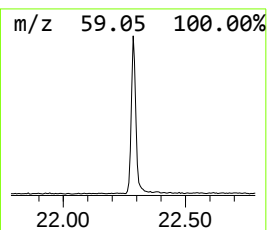
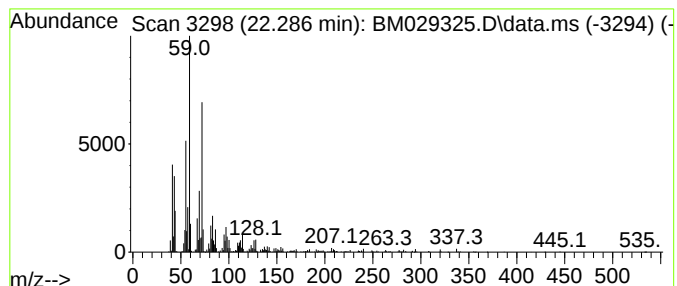
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.286	14.24 ng	976499	Chrysene-d12	21.244

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
4		4-Cyclohexylbutyramide	169	C10H19NO	004441-62-7	59
5		Hexadecanamide	255	C16H33NO	000629-54-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029325.D
Acq On : 02 Apr 2021 17:47
Operator : CG/JU
Sample : M1874-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB16(26-27)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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...	2.946	18.0	ng	582903	1	7.698	648376	20.0
unknown2.987	2.987	3.5	ng	115124	1	7.698	648376	20.0
2-Pentanone, 4-...	4.846	2.6	ng	84991	1	7.698	648376	20.0
Tridecanoic acid	17.974	2.7	ng	160301	4	17.068	1175700	20.0
9-Eicosene, (E)-	20.968	9.6	ng	657811	5	21.244	1371510	20.0
9-Octadecenamid...	22.286	14.2	ng	976499	5	21.244	1371510	20.0