LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029266.D
Acq On : 30 Mar 2021 04:24
Operator : CG/JU
Sample : M1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : EL-510-STREET-LEVEL

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-BM032621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	18	22	26	rBV	464701	555222	10.16%	1.625%
2	3.057	26	29	37	rVB	89584	111931	2.05%	0.328%
3	4.904	337	343	352	rBV	166423	239859	4.39%	0.702%
4	5.363	414	421	433	rBV	1793540	2629809	48.14%	7.698%
5	6.934	680	688	702	rBV	1795792	2871620	52.57%	8.406%
6	7.757	821	828	835	rBV	570942	894558	16.38%	2.619%
7	8.904	1015	1023	1033	rBV	1104686	1849695	33.86%	5.415%
8	10.539	1293	1301	1308	rBV	735614	1235653	22.62%	3.617%
9	13.004	1713	1720	1730	rBV	2594284	3795895	69.49%	11.112%
10	13.839	1856	1862	1873	rVB	74592	115440	2.11%	0.338%
11	14.215	1920	1926	1935	rBV2	24067	57003	1.04%	0.167%
12	14.292	1935	1939	1945	rVB	42144	59163	1.08%	0.173%
13	14.380	1948	1954	1963	rBV2	1037115	1564648	28.64%	4.580%
14	15.868	2201	2207	2214	rBV	1923003	2697660	49.38%	7.897%
15	16.068	2235	2241	2249	rBV	377277	542311	9.93%	1.588%
16	17.121	2414	2420	2426	rBV	1327581	1821508	33.34%	5.332%
17	18.021	2568	2573	2589	rBV	570152	908758	16.64%	2.660%
18	19.180	2762	2770	2783	rBV4	322710	1108761	20.30%	3.246%
19	19.297	2786	2790	2804	rVB	375802	602091	11.02%	1.763%
20	19.739	2860	2865	2871	rBV	4344126	5462653	100.00%	15.991%
21	21.003	3076	3080	3085	rBV	715966	861141	15.76%	2.521%
22	21.286	3124	3128	3133	rBV	1622173	2046291	37.46%	5.990%
23	23.527	3503	3509	3518	rVB2	1127232	2128681	38.97%	6.231%

Sum of corrected areas: 34160351

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Instrument :
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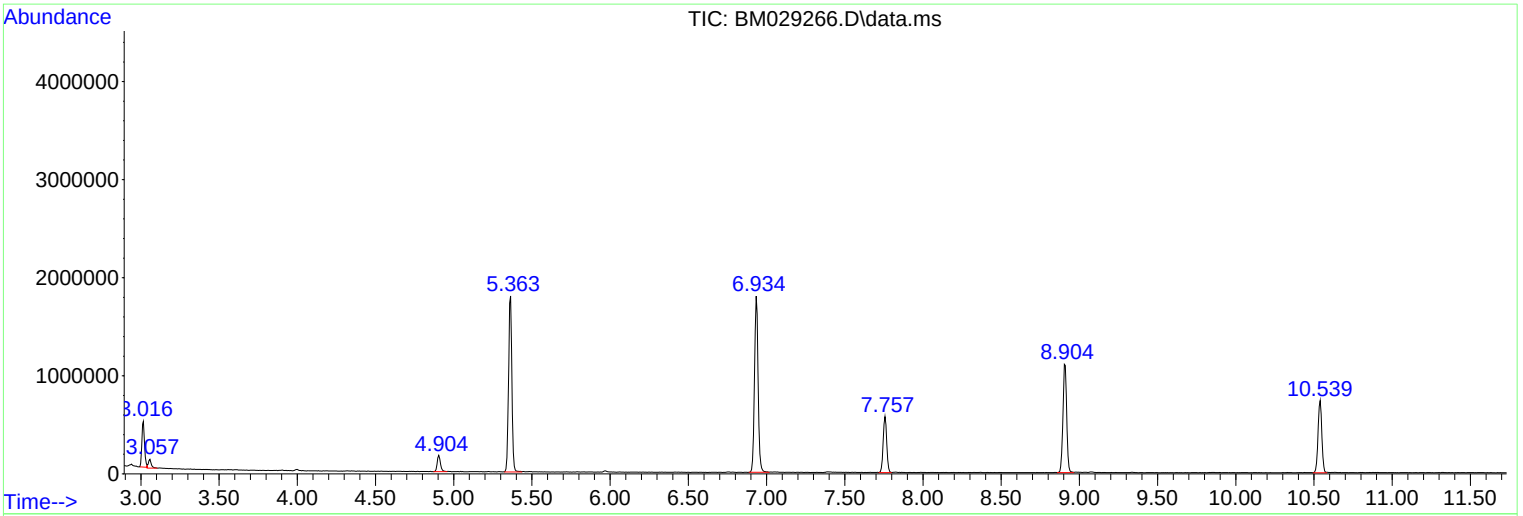
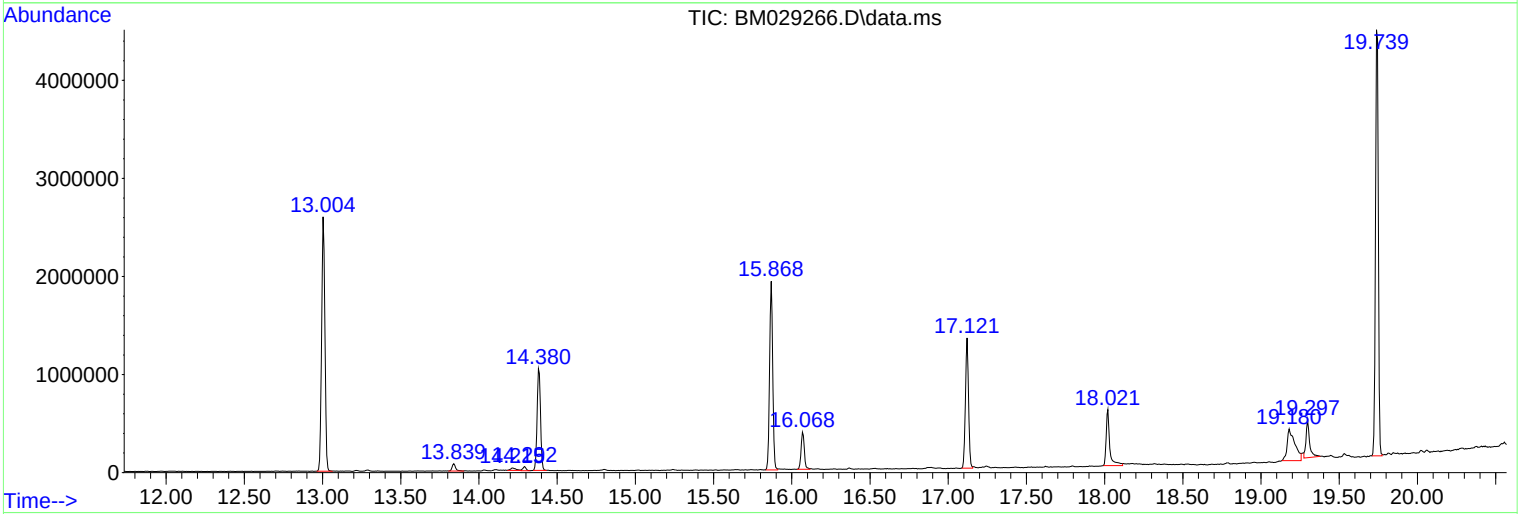
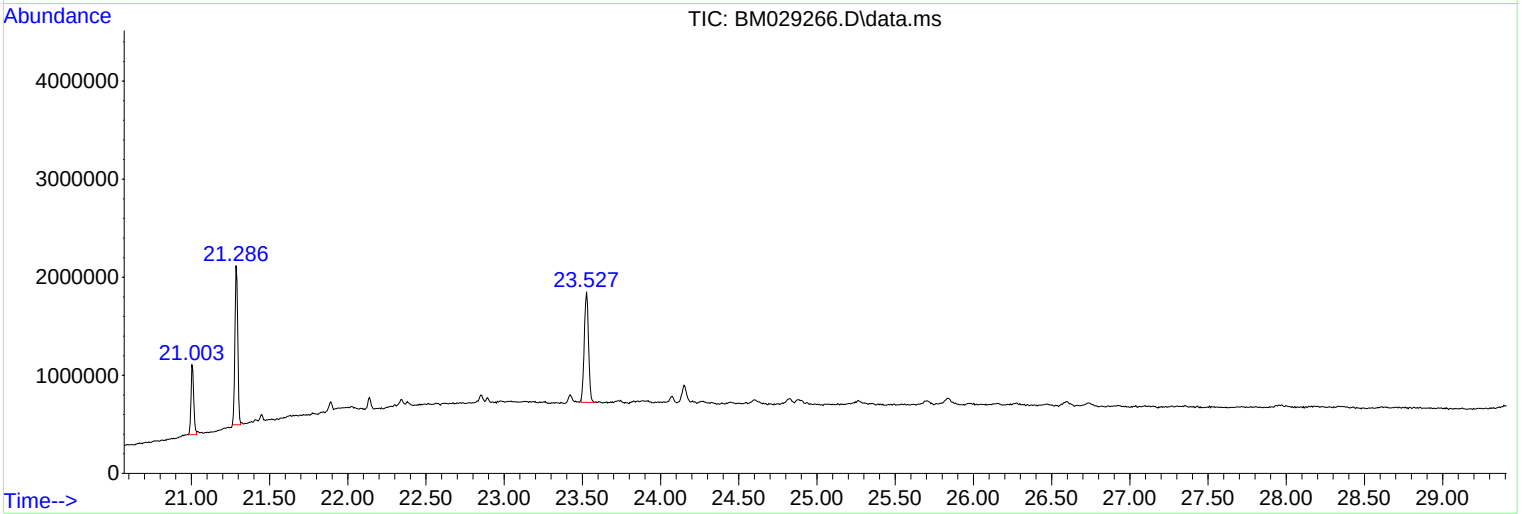
ClientSampleId :
EL-510-STREET-LEVEL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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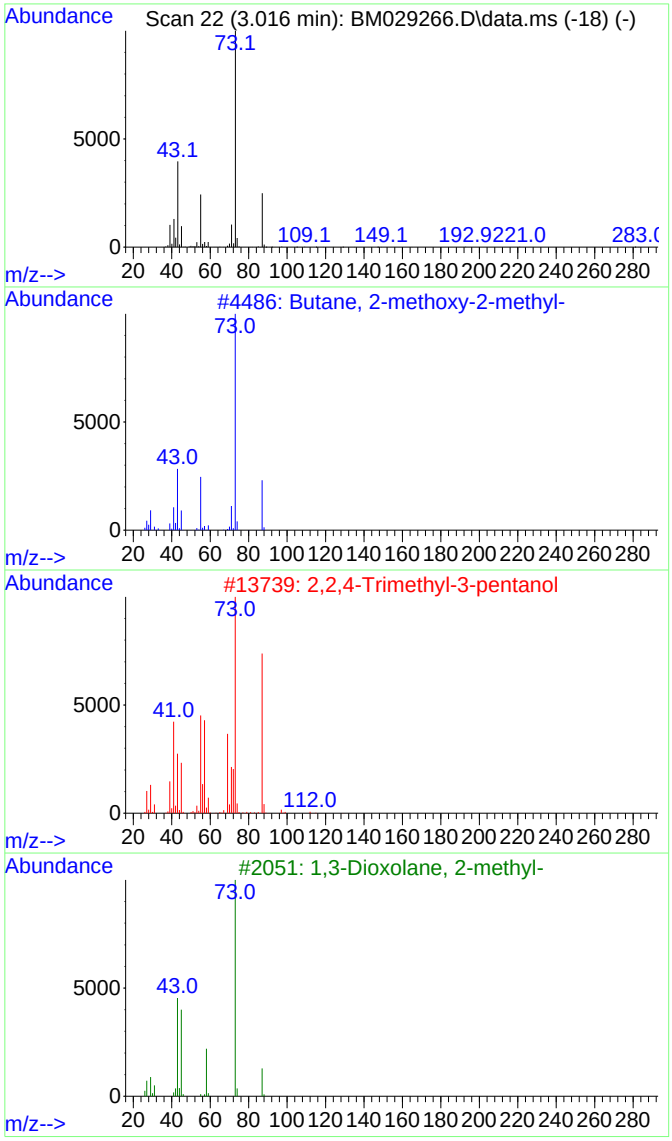
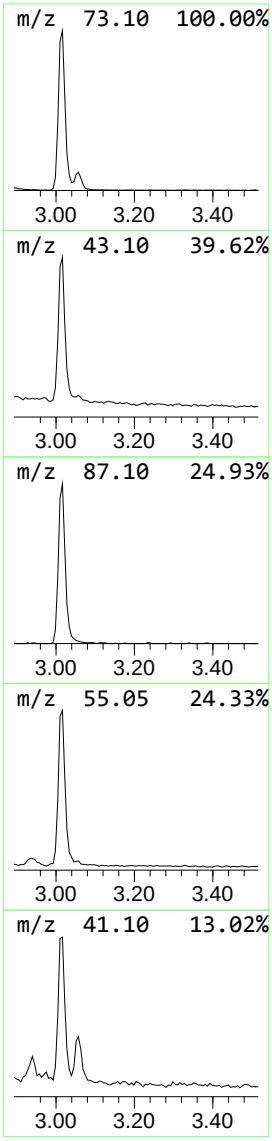
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	12.41 ng	555222	1,4-Dichlorobenzene-d4	7.757

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16





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Sample : M1821-02
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
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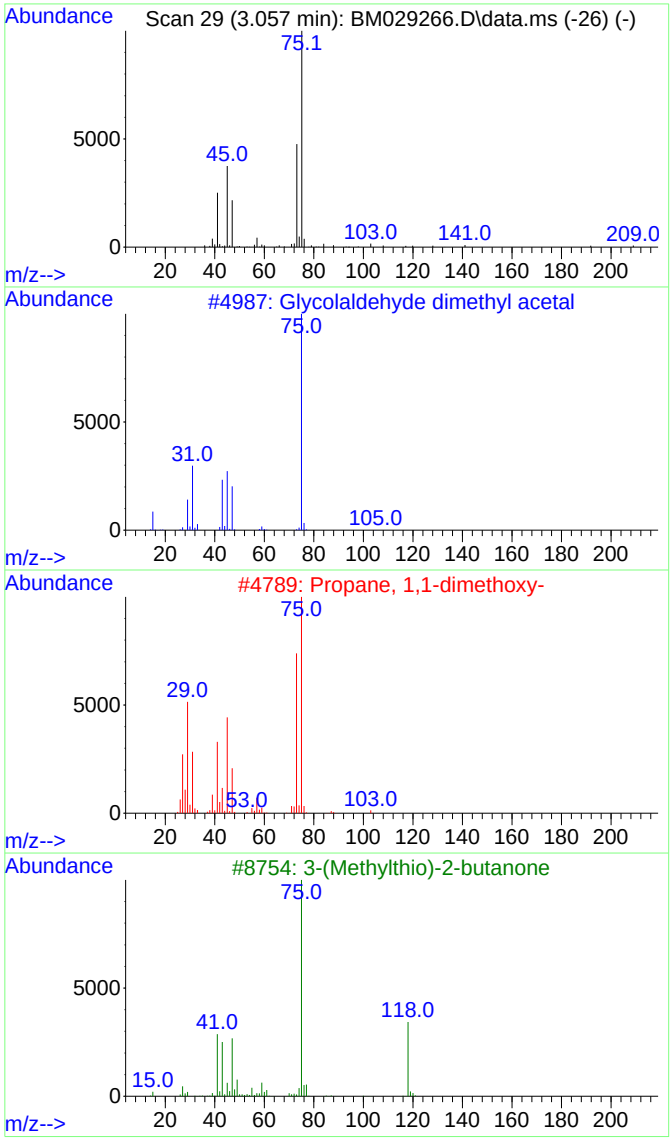
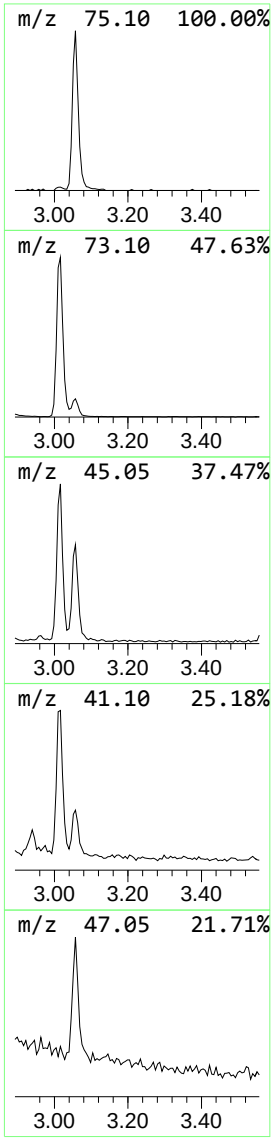
****
Peak Number 2 Glycolaldehyde dimethyl acetal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.057	2.50 ng	111931	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
2	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
3	3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	38
4	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	36
5	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	9





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Sample : M1821-02
Misc :
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Instrument :
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ClientSampleId :
EL-510-STREET-LEVEL

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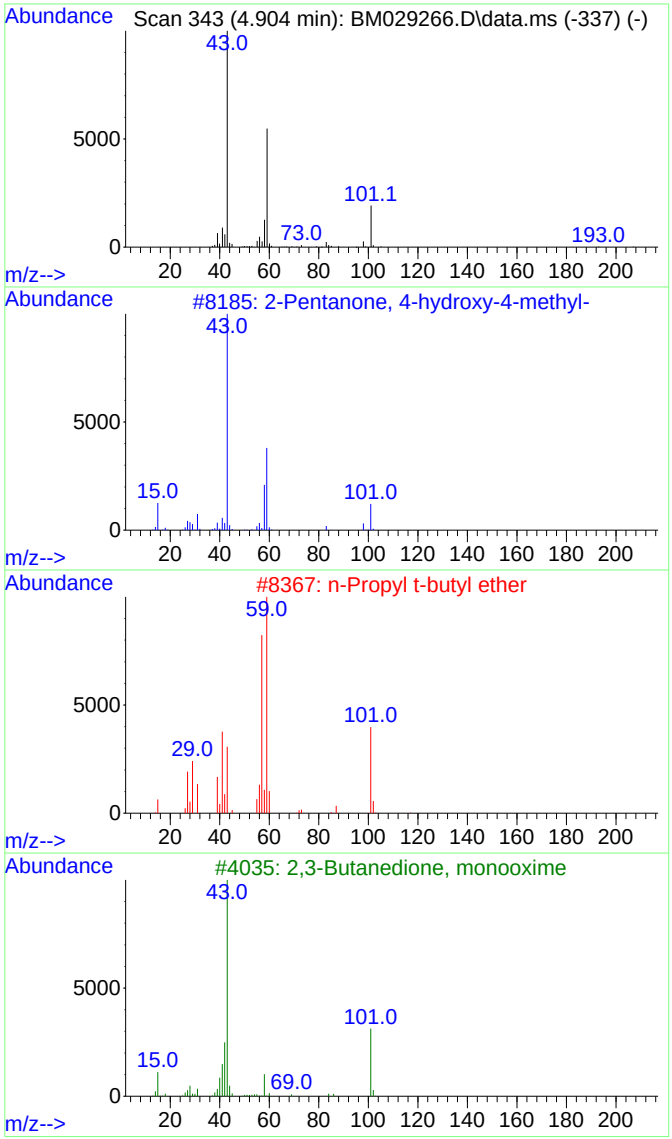
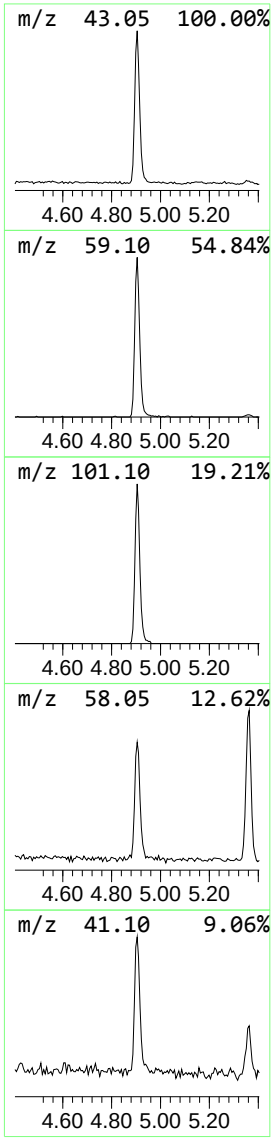
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	5.36 ng	239859	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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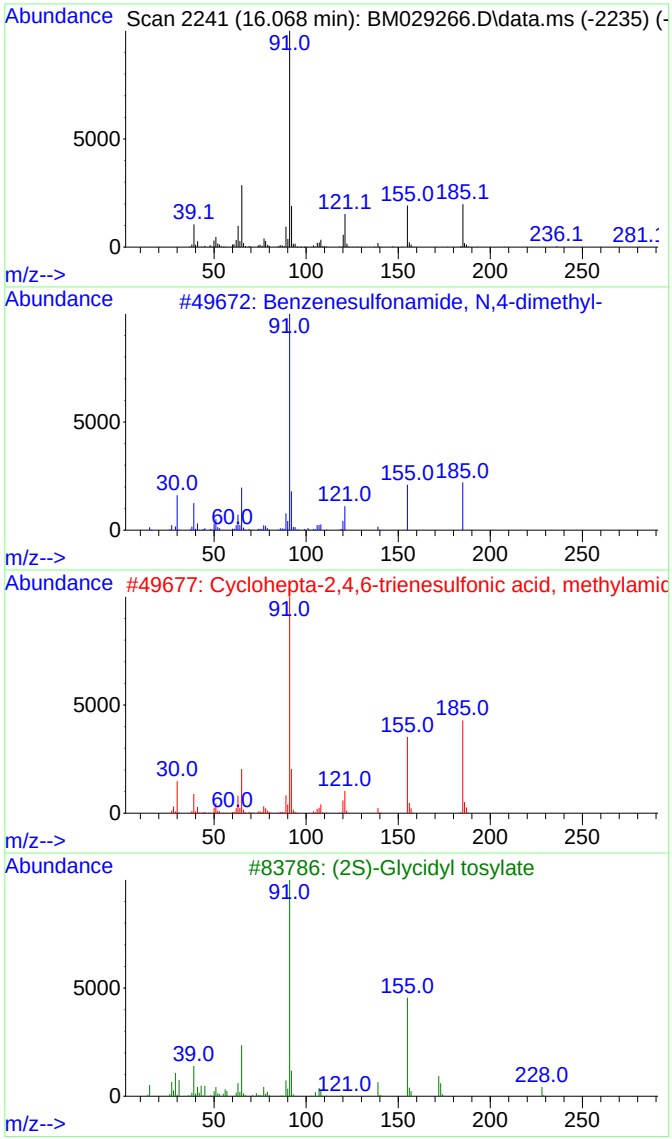
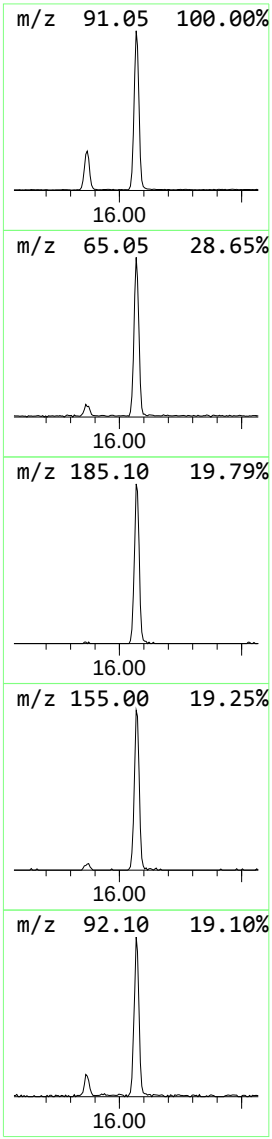
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.068	5.95 ng	542311	Phenanthrene-d10	17.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	94
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	50
3	(2S)-Glycidyl tosylate	228	C10H12O4S	070987-78-9	47
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	47





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Misc :
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Instrument : BNA_M
ClientSampleId : EL-510-STREET-LEVEL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

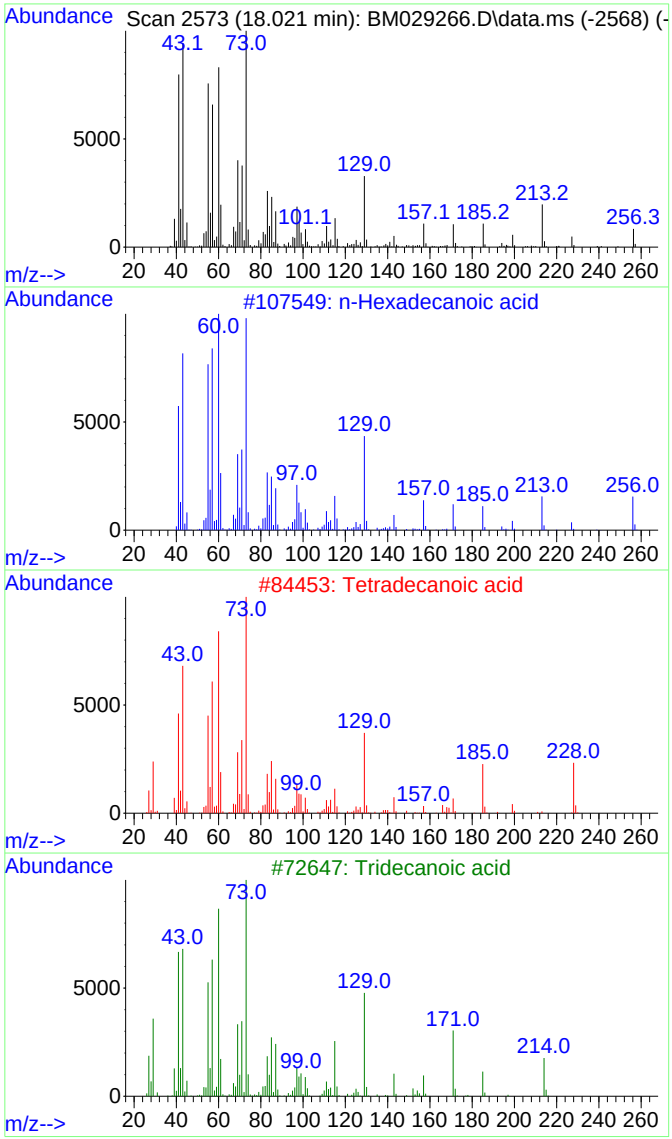
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

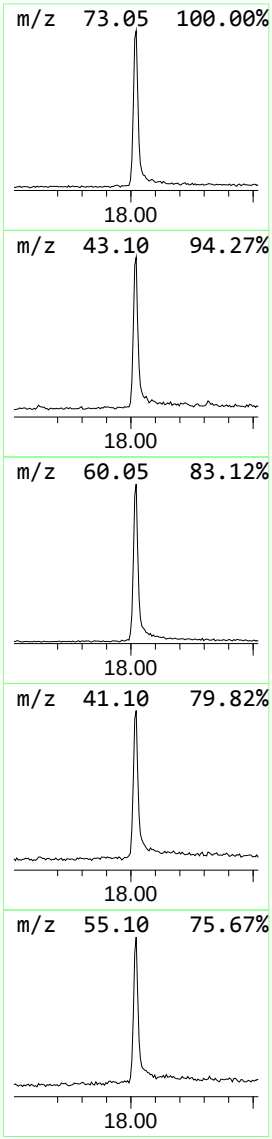
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	9.98 ng	908758	Phenanthrene-d10	17.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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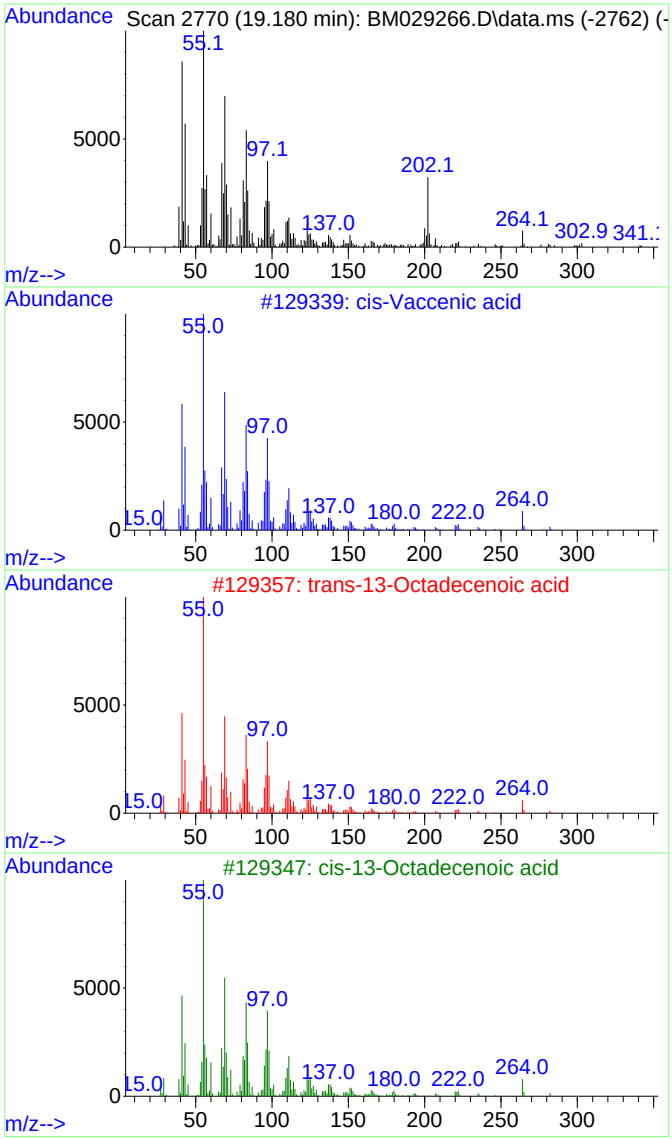
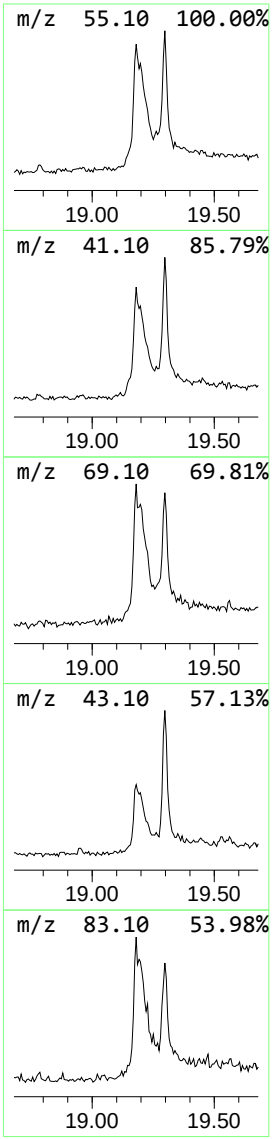
****

Peak Number 6 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.180	12.17 ng	1108760	Phenanthrene-d10	17.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	96
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
5	Oleic Acid	282	C18H34O2	000112-80-1	94





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

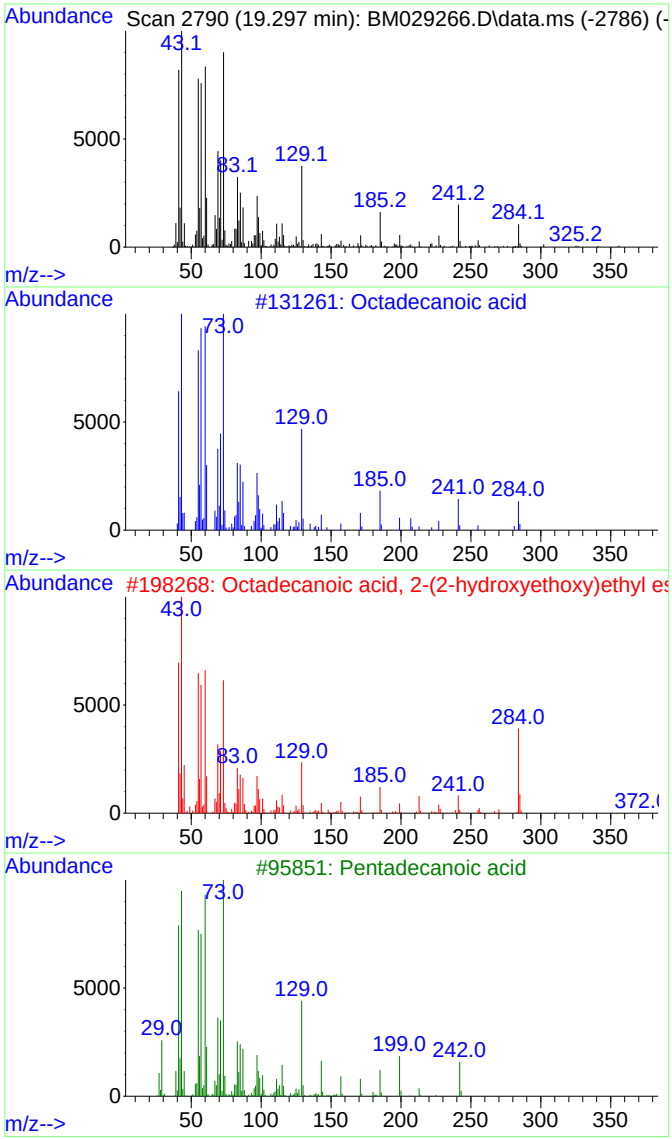
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

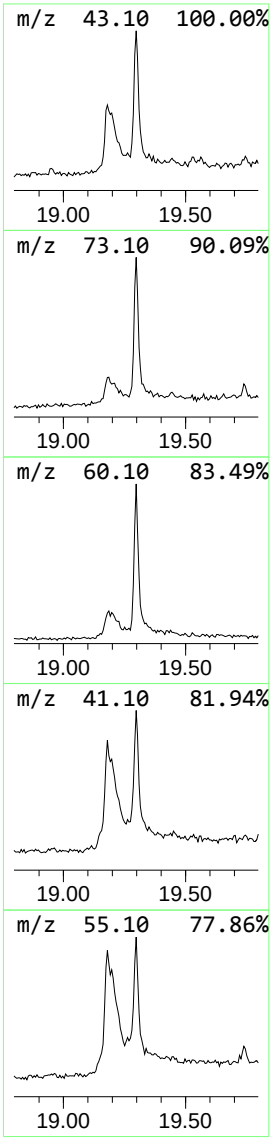
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.297	5.88 ng	602091	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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TIC Library : C:\DATABASE\NIST11.L
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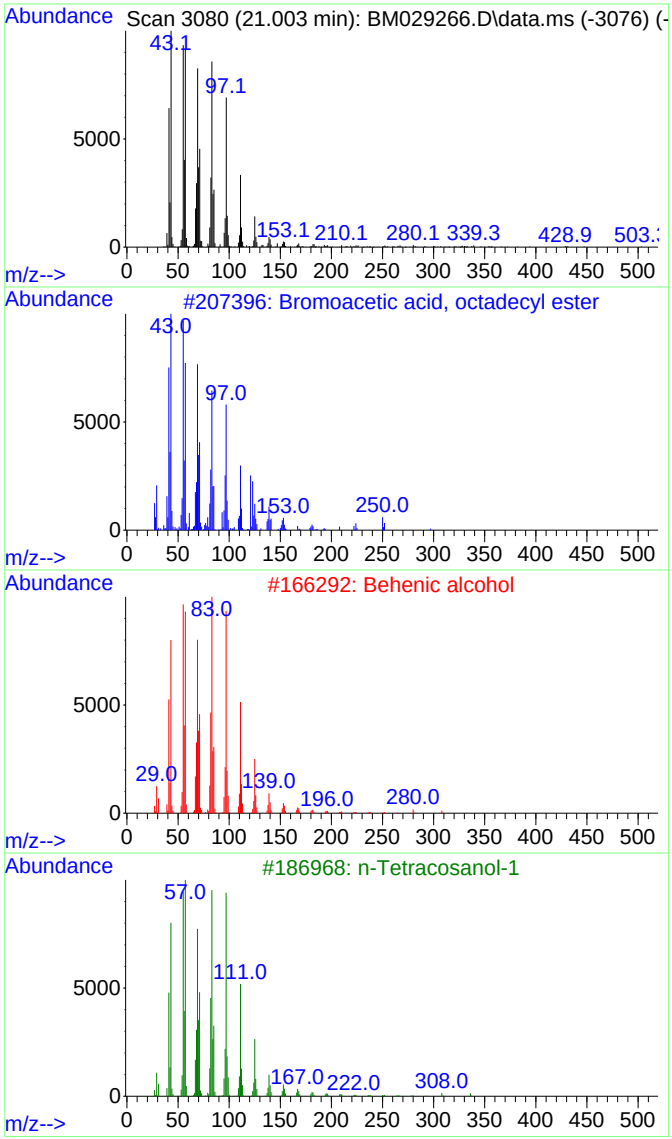
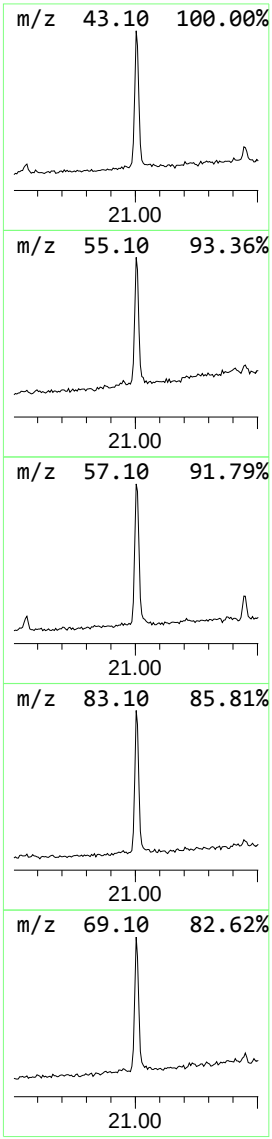
****

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.003	8.42 ng	861141	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.016	12.4	ng	555222	1	7.757	894558	20.0
Glycolaldehyde ...	3.057	2.5	ng	111931	1	7.757	894558	20.0
2-Pentanone, 4-...	4.904	5.4	ng	239859	1	7.757	894558	20.0
Benzenesulfonam...	16.068	6.0	ng	542311	4	17.121	1821510	20.0
n-Hexadecanoic ...	18.021	10.0	ng	908758	4	17.121	1821510	20.0
cis-Vaccenic acid	19.180	12.2	ng	1108760	4	17.121	1821510	20.0
Octadecanoic acid	19.297	5.9	ng	602091	5	21.286	2046290	20.0
Bromoacetic aci...	21.003	8.4	ng	861141	5	21.286	2046290	20.0