LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100522\
Data File : BM036834.D
Acq On : 05 Oct 2022 13:10
Operator : CG/JU
Sample : N4785-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PT-ACIDS-WP

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-BM100322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.828	121	126	133	rBV	303502	365349	2.17%	0.179%
2	4.446	225	231	243	rBV	1051068	1358719	8.07%	0.665%
3	5.063	328	336	347	rBV	1595083	2322632	13.80%	1.136%
4	5.522	407	414	426	rBV	6819110	9620652	57.15%	4.706%
5	7.134	678	688	690	rBV	6481572	11320075	67.25%	5.538%
6	7.157	690	692	719	rVB	5839988	7208349	42.82%	3.526%
7	7.528	747	755	773	rBV	5397011	8357735	49.65%	4.088%
8	7.963	821	829	838	rBV	1201339	1869640	11.11%	0.915%
9	8.416	897	906	923	rBV	8856607	13951095	82.88%	6.825%
10	8.734	952	960	972	rBV	3587358	5571255	33.10%	2.725%
11	9.134	1020	1028	1036	rBV	4016168	6216886	36.93%	3.041%
12	9.887	1148	1156	1161	rBV	2586819	4252778	25.26%	2.080%
13	9.945	1161	1166	1181	rVB	3007289	4732766	28.12%	2.315%
14	10.422	1238	1247	1264	rBV	8381999	13388794	79.54%	6.550%
15	10.775	1296	1307	1318	rVB	1707876	2757348	16.38%	1.349%
16	10.951	1329	1337	1349	rBV	4040476	6658531	39.56%	3.257%
17	12.057	1515	1525	1546	rBV	9508901	14918014	88.62%	7.298%
18	13.034	1683	1691	1697	rBV	9563986	13891253	82.52%	6.795%
19	13.098	1697	1702	1717	rVV	1947003	3018088	17.93%	1.476%
20	13.228	1717	1724	1737	rVB	9965316	13554193	80.52%	6.630%
21	14.598	1950	1957	1968	rBV	2308912	3358753	19.95%	1.643%
22	14.710	1968	1976	1985	rBV	4360947	6013273	35.72%	2.942%
23	14.810	1985	1993	2015	rVB	6598270	10332443	61.38%	5.054%
24	15.716	2140	2147	2166	rBV	2013730	2603846	15.47%	1.274%
25	16.080	2202	2209	2227	rBV	6814445	9328347	55.42%	4.563%
26	17.333	2415	2422	2430	rBV	2687994	3753604	22.30%	1.836%
27	19.951	2861	2867	2876	rBV	14131848	16833379	100.00%	8.235%
28	20.709	2992	2996	3001	rBV	543291	644260	3.83%	0.315%
29	21.504	3127	3131	3141	rBV2	2688304	3456264	20.53%	1.691%
30	23.921	3536	3542	3553	rVB	1417746	2764843	16.42%	1.353%

Sum of corrected areas: 204423164

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Instrument :
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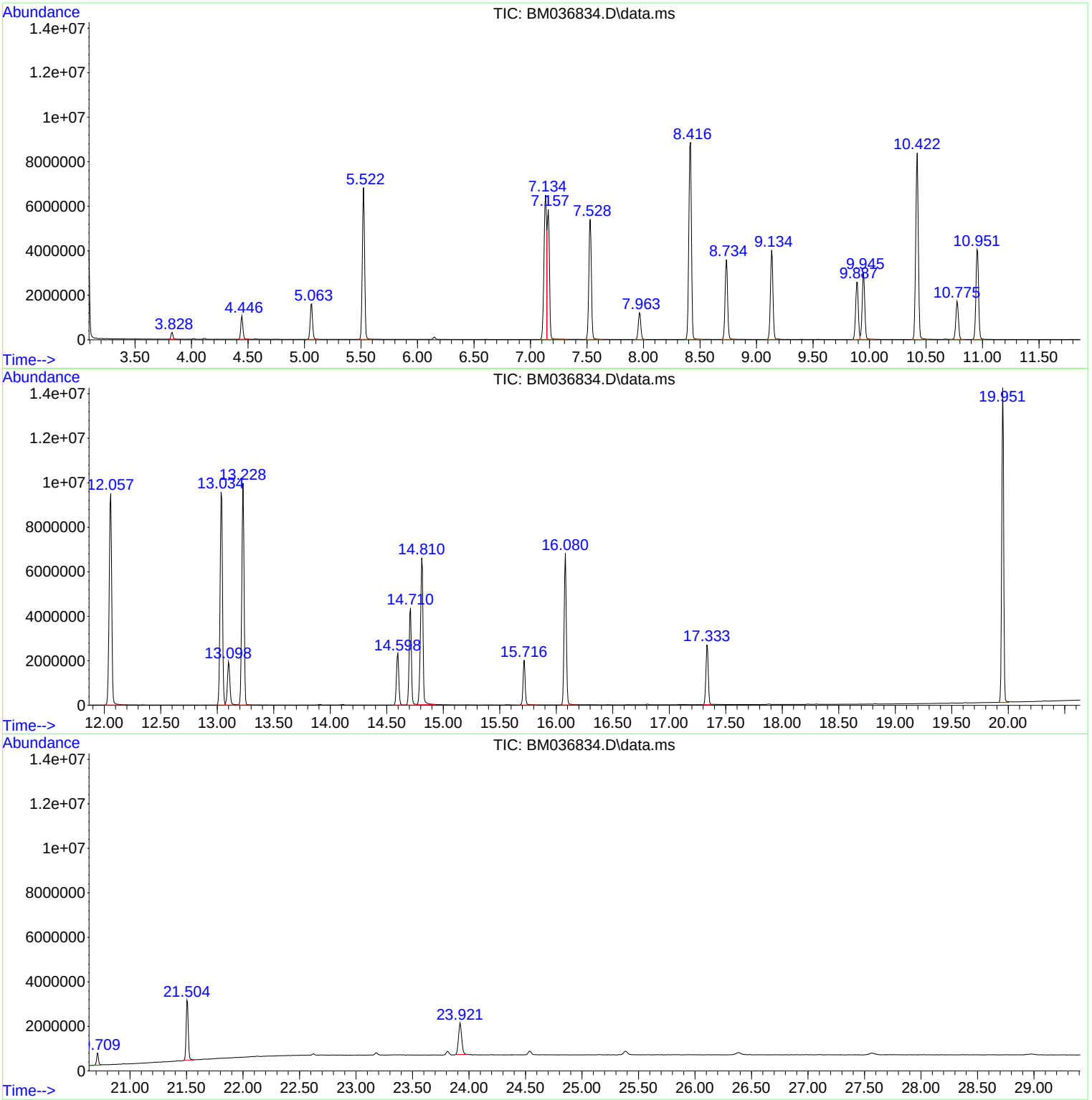
ClientSampleId :
PT-ACIDS-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.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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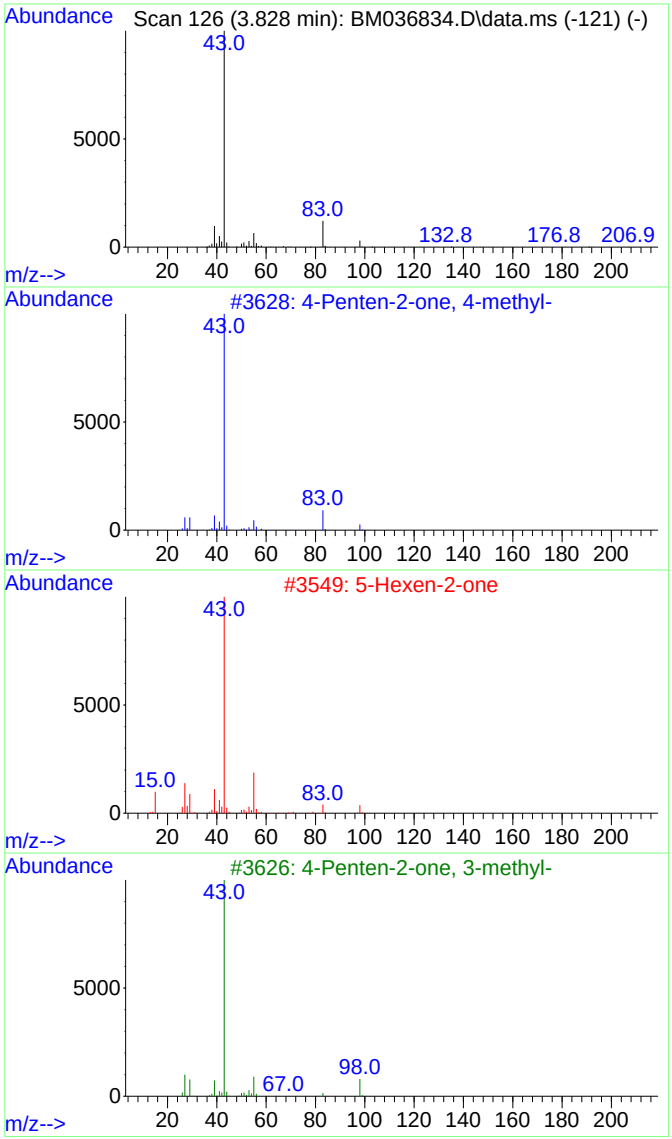
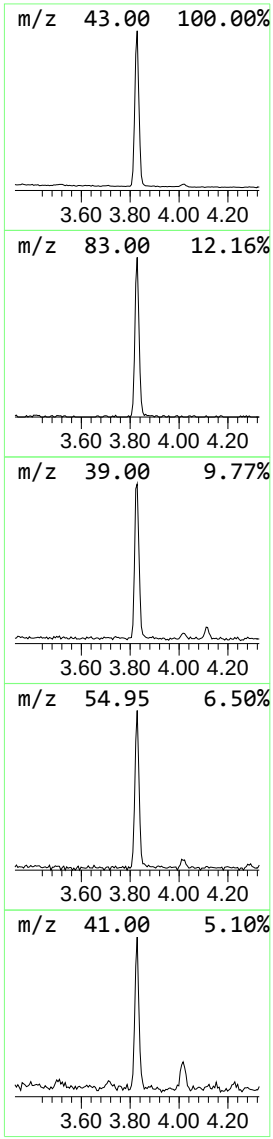
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.828	3.91 ng	365349	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	53
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	40
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





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Sample : N4785-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PT-ACIDS-WP

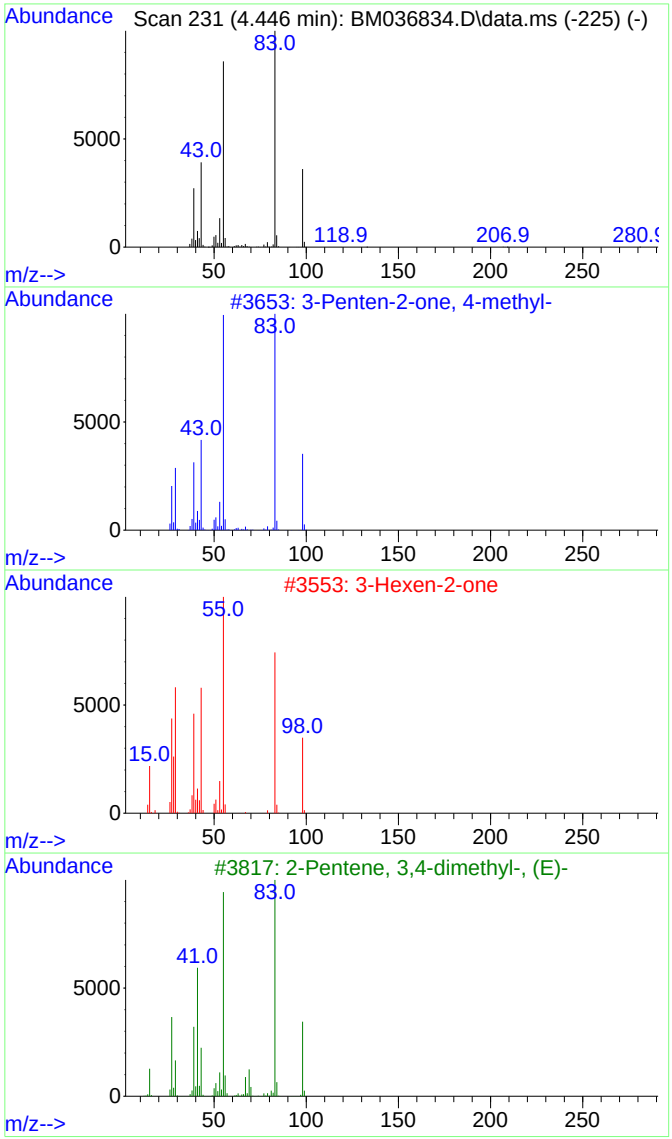
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

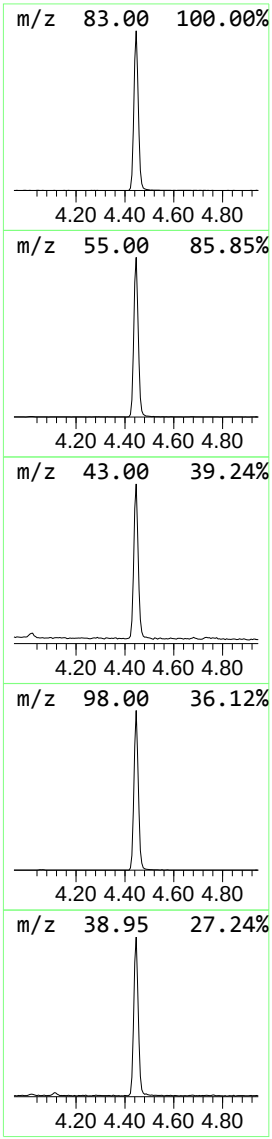
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	14.53 ng	1358720	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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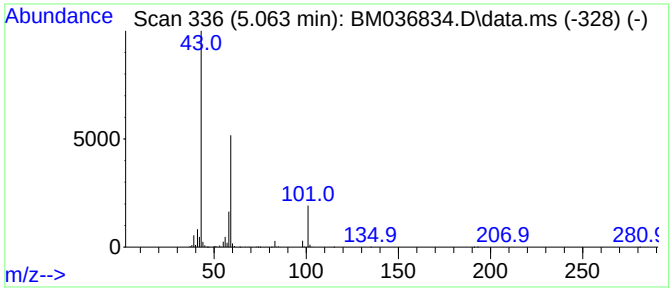
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

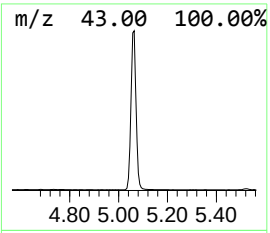
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

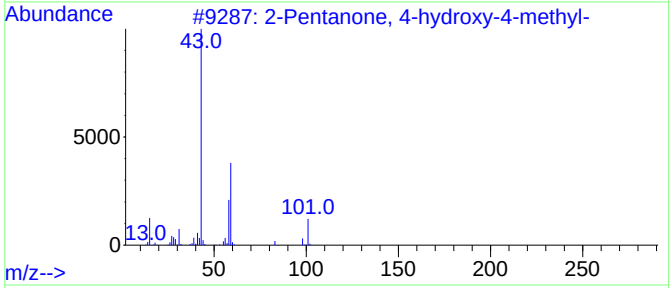
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

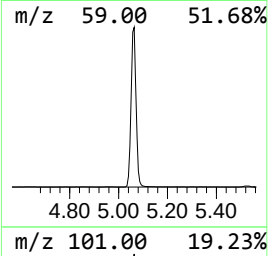
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	24.85 ng	2322630	1,4-Dichlorobenzene-d4	7.963

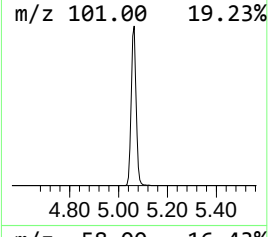
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

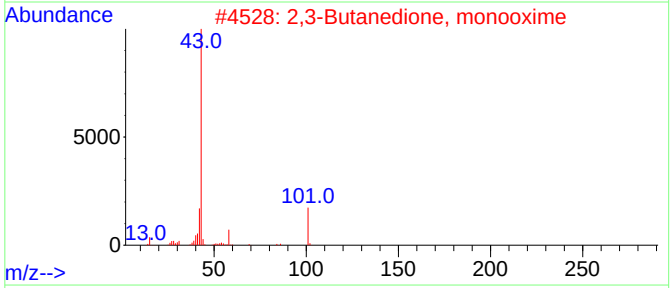


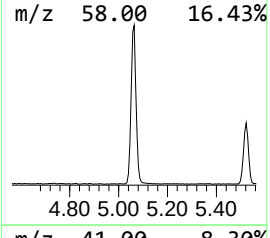


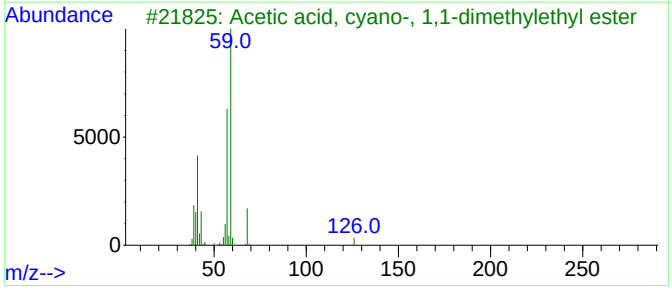


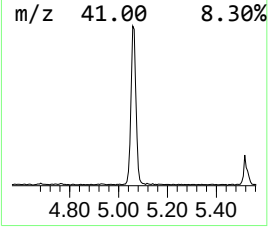












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

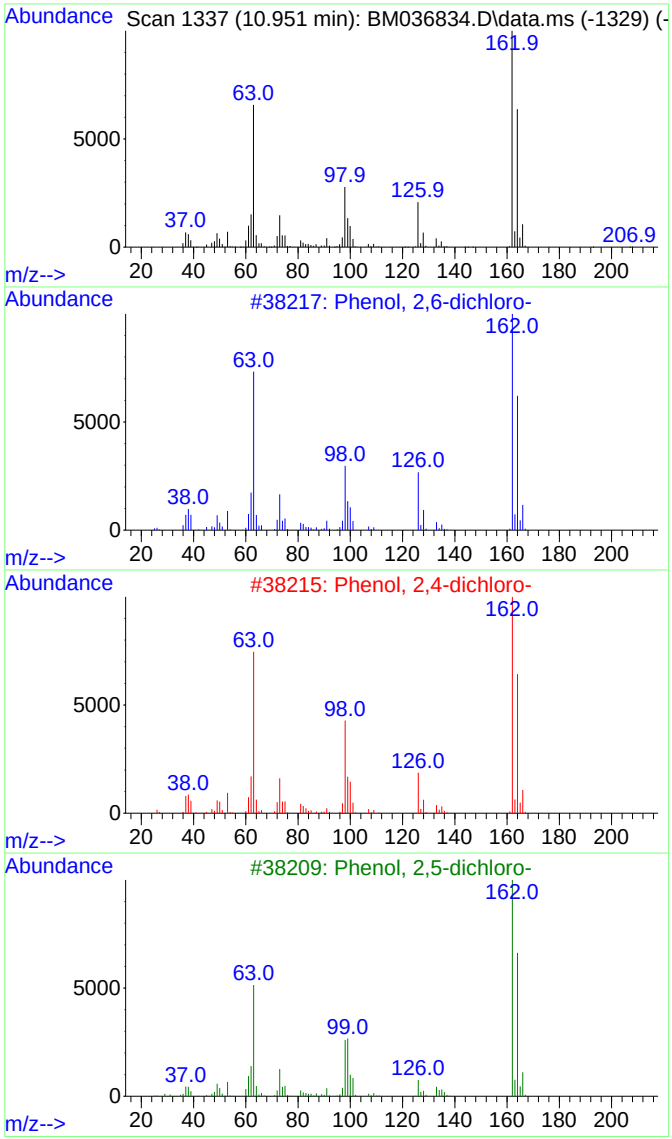
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

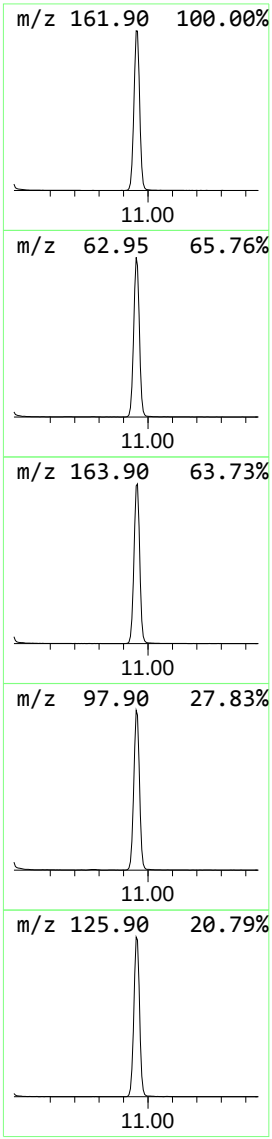
****

Peak Number 4 Phenol, 2,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.951	48.30 ng	6658530	Naphthalene-d8	10.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	98
2	Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	96
3	Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	94
4	Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	93
5	Phenol, 3,5-dichloro-	162	C6H4Cl2O	000591-35-5	64





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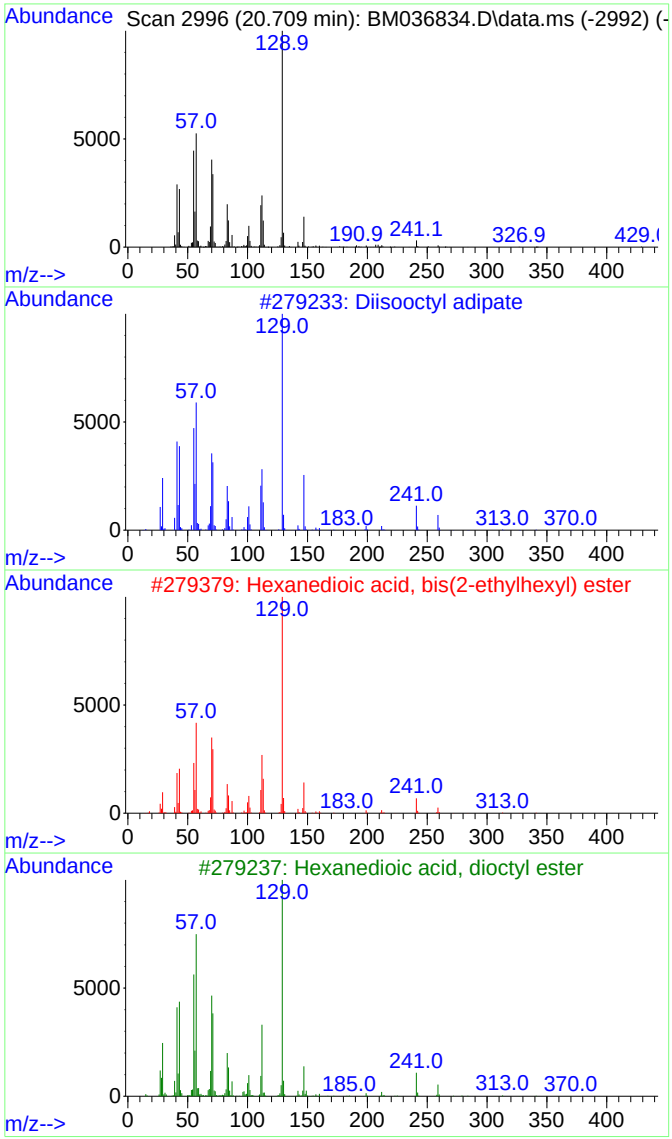
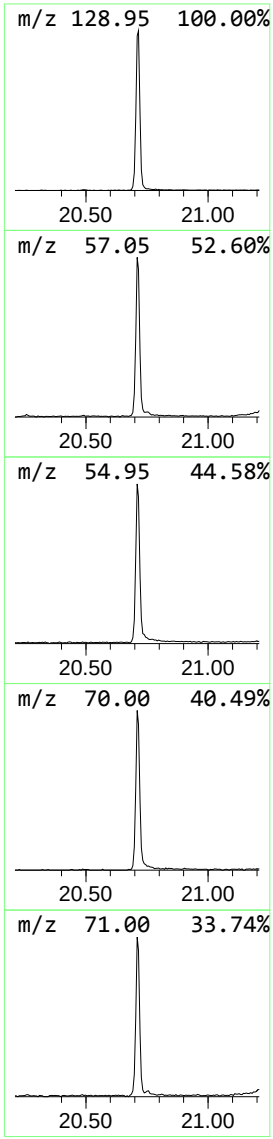
****

Peak Number 5 Diisooctyl adipate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.709	3.73 ng	644260	Chrysene-d12	21.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
4	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	50
5	Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	43





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Penten-2-one,...	3.828	3.9	ng	365349	1	7.963	1869640	20.0
3-Penten-2-one,...	4.446	14.5	ng	1358720	1	7.963	1869640	20.0
2-Pentanone, 4-...	5.063	24.9	ng	2322630	1	7.963	1869640	20.0
Phenol, 2,6-dic...	10.951	48.3	ng	6658530	2	10.775	2757350	20.0
Diisooctyl adipate	20.709	3.7	ng	644260	5	21.503	3456260	20.0