LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121021\
Data File : BP008359.D
Acq On : 11 Dec 2021 01:37
Operator : CG/JU
Sample : M4990-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R3-COMP

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.022	3	6	18	rVB2	198124	242448	8.02%	1.223%
2	3.964	161	166	172	rVB	31662	47841	1.58%	0.241%
3	4.293	217	222	226	rBV	40764	56701	1.87%	0.286%
4	4.516	256	260	267	rVB	27863	41308	1.37%	0.208%
5	4.887	318	323	333	rBV	329131	462062	15.28%	2.330%
6	5.358	397	403	409	rBV	1107307	1676221	55.43%	8.452%
7	5.775	468	474	479	rBV	25588	41969	1.39%	0.212%
8	6.952	663	674	695	rBV	955589	1701349	56.26%	8.579%
9	7.757	803	811	821	rBV	331006	534651	17.68%	2.696%
10	8.922	1002	1009	1026	rVB	642742	1105618	36.56%	5.575%
11	10.551	1277	1286	1293	rBV	324846	582591	19.26%	2.938%
12	11.987	1523	1530	1535	rBV2	18132	31389	1.04%	0.158%
13	13.028	1699	1707	1723	rBV	1416835	2075854	68.64%	10.467%
14	13.239	1738	1743	1746	rBV2	39072	53655	1.77%	0.271%
15	14.316	1921	1926	1932	rBV	32693	46890	1.55%	0.236%
16	14.410	1935	1942	1949	rVV	466308	709711	23.47%	3.579%
17	14.475	1949	1953	1961	rVB3	18265	34887	1.15%	0.176%
18	15.275	2085	2089	2095	rVB	25354	33606	1.11%	0.169%
19	15.469	2117	2122	2132	rVB5	19462	42155	1.39%	0.213%
20	15.839	2180	2185	2190	rBV	78465	98017	3.24%	0.494%
21	15.910	2191	2197	2206	rBV	886211	1377449	45.55%	6.946%
22	16.139	2232	2236	2245	rVB2	32219	67040	2.22%	0.338%
23	16.939	2369	2372	2376	rVV	33995	37475	1.24%	0.189%
24	16.992	2378	2381	2390	rVB3	30819	47380	1.57%	0.239%
25	17.104	2396	2400	2405	rVB2	23688	32544	1.08%	0.164%
26	17.175	2406	2412	2416	rBV	588367	831384	27.49%	4.192%
27	17.216	2416	2419	2424	rVB	131493	176786	5.85%	0.891%
28	17.304	2429	2434	2440	rVB2	76428	141317	4.67%	0.713%
29	17.469	2458	2462	2473	rVB2	32197	61167	2.02%	0.308%
30	17.686	2495	2499	2502	rBV	32202	38874	1.29%	0.196%
31	17.833	2520	2524	2531	rVB2	63457	98640	3.26%	0.497%
32	18.098	2563	2569	2573	rVB2	47873	97971	3.24%	0.494%
33	18.139	2573	2576	2580	rBV	54687	64699	2.14%	0.326%
34	18.233	2588	2592	2596	rBV3	38734	58922	1.95%	0.297%
35	18.357	2610	2613	2617	rBV	48722	63205	2.09%	0.319%
36	18.533	2640	2643	2647	rBV	25876	39194	1.30%	0.198%

LSC Area Percent Report

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Acq On : 11 Dec 2021 01:37
Operator : CG/JU
Sample : M4990-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R3-COMP

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.810	2687	2690	2695	rBV2	27452	46113	1.52%	0.233%
38	18.974	2715	2718	2721	rBV	43849	43390	1.43%	0.219%
39	19.198	2751	2756	2761	rBV	306981	405048	13.39%	2.042%
40	19.251	2762	2765	2770	rVB2	61740	77898	2.58%	0.393%
41	19.551	2809	2816	2825	rVB	248026	447929	14.81%	2.259%
42	19.751	2845	2850	2855	rVB	2557872	3024113	100.00%	15.249%
43	20.998	3059	3062	3072	rVB3	264782	411875	13.62%	2.077%
44	21.192	3093	3095	3099	rVB	113366	112497	3.72%	0.567%
45	21.280	3105	3110	3114	rBV2	877761	1288120	42.59%	6.495%
46	23.662	3510	3515	3522	rBV2	586171	1122187	37.11%	5.658%

Sum of corrected areas: 19832140

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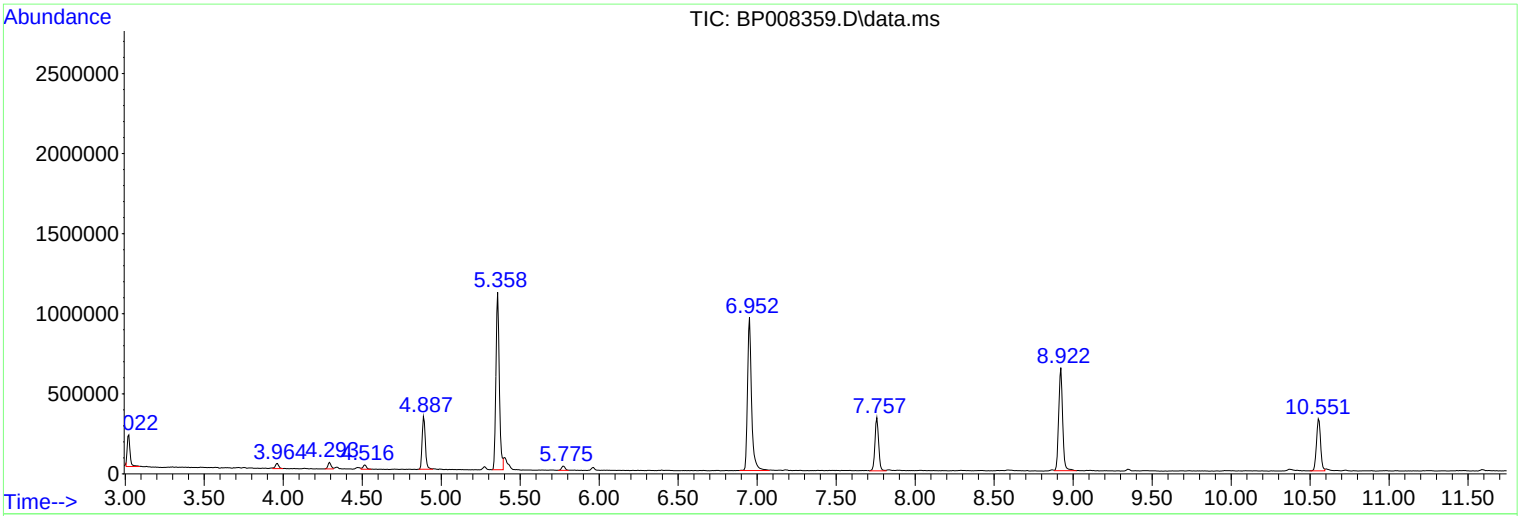
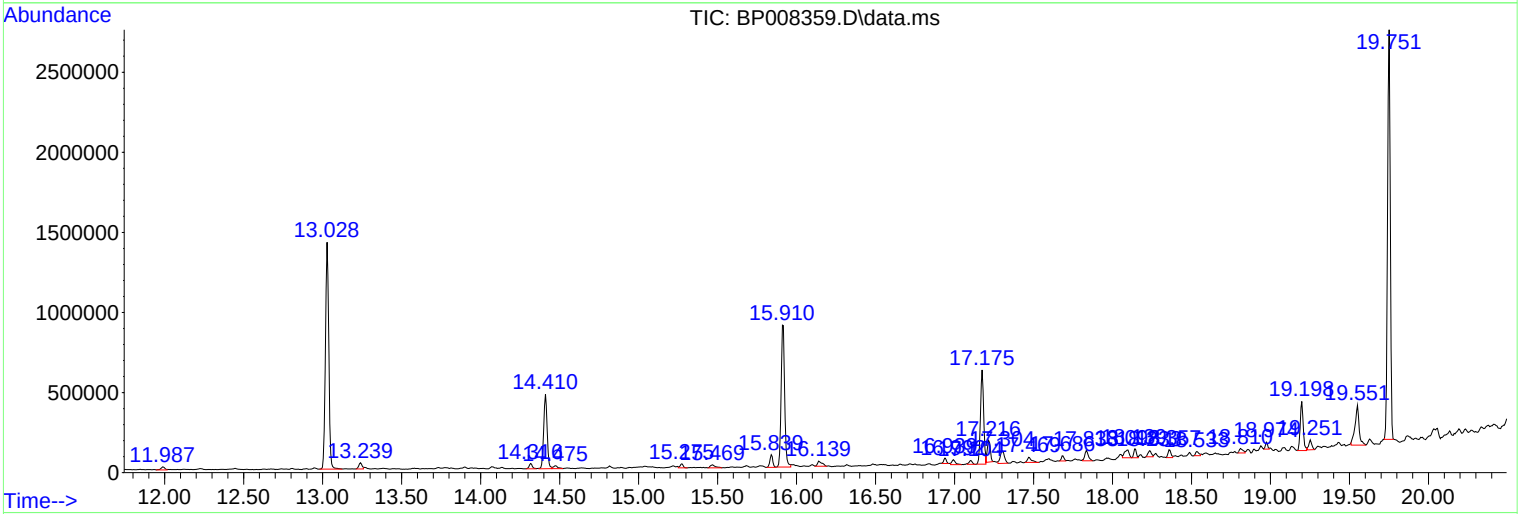
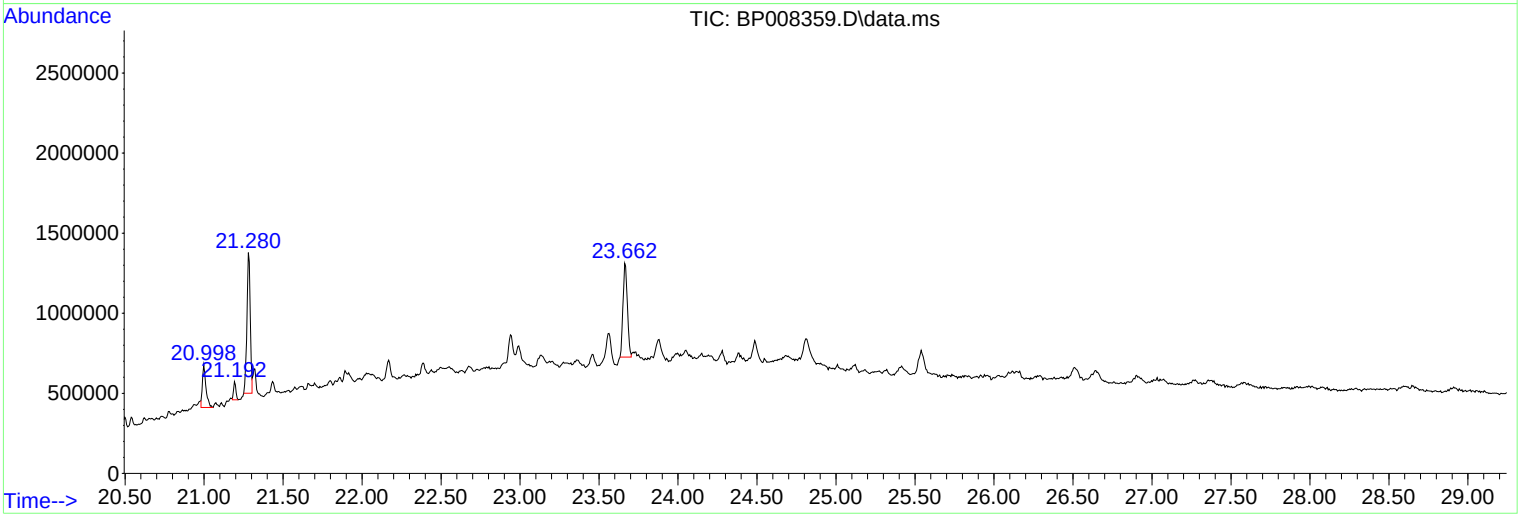
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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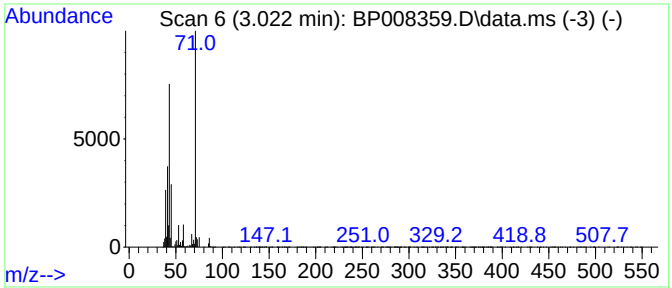
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

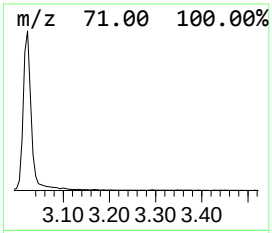
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

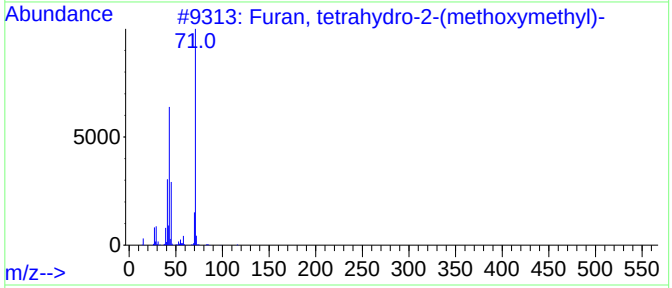
****
Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 2

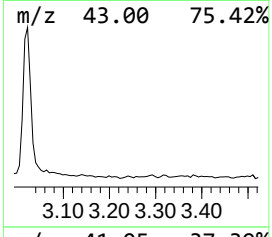
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.022	9.07 ng	242448	1,4-Dichlorobenzene-d4	7.757

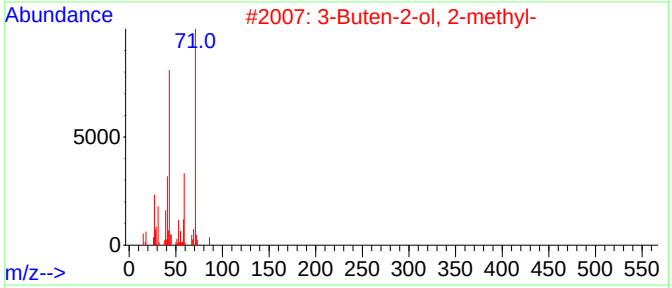
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
3	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	59
4	3-Penten-2-ol	86	C5H10O	001569-50-2	59
5	2-Tetrahydrofurfuryl isothiocyanate	143	C6H9NOS	036810-87-4	53

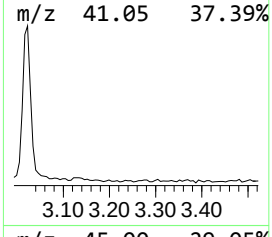


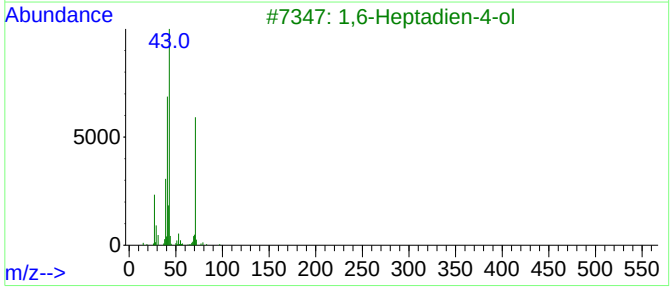


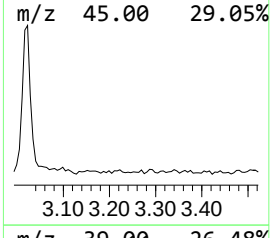


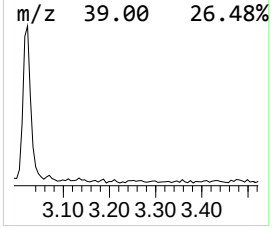












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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R3-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

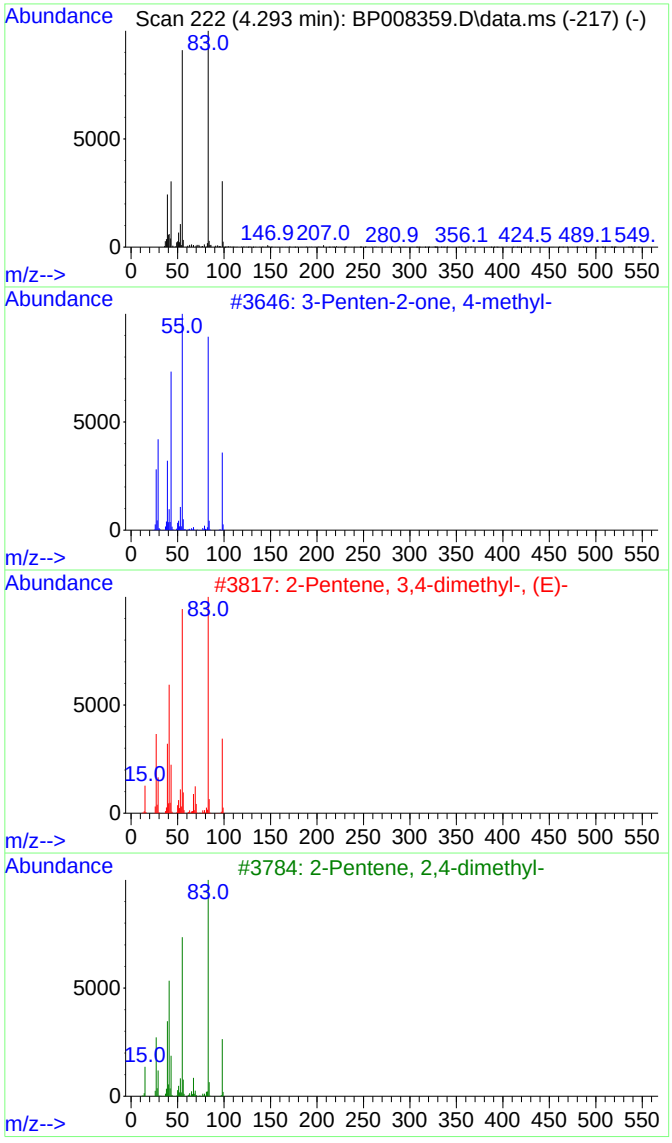
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

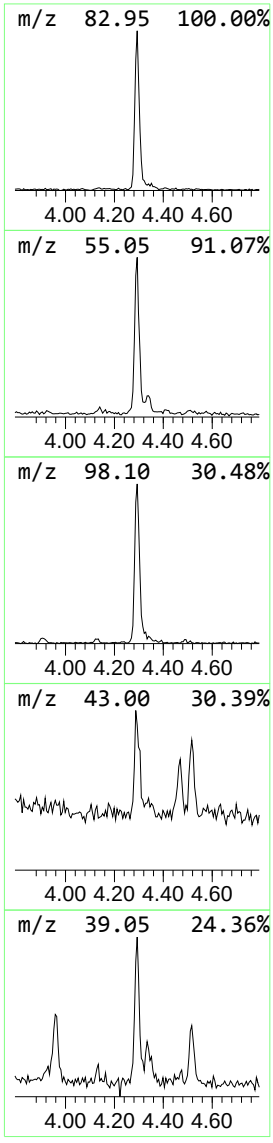
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.293	2.12 ng	56701	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	78
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





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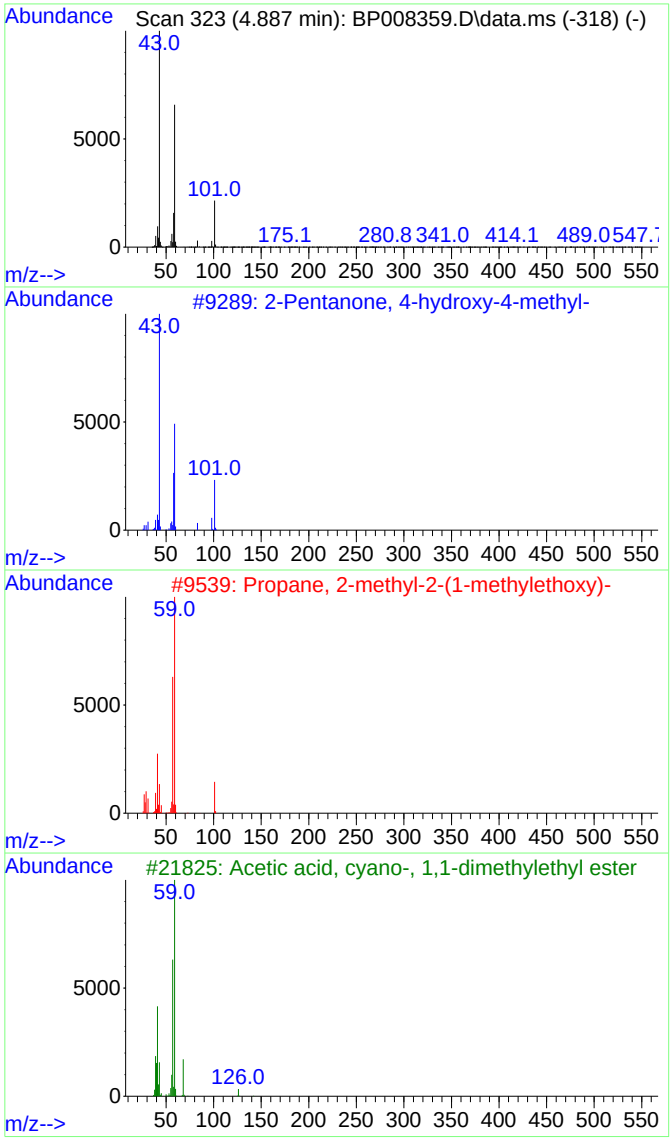
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

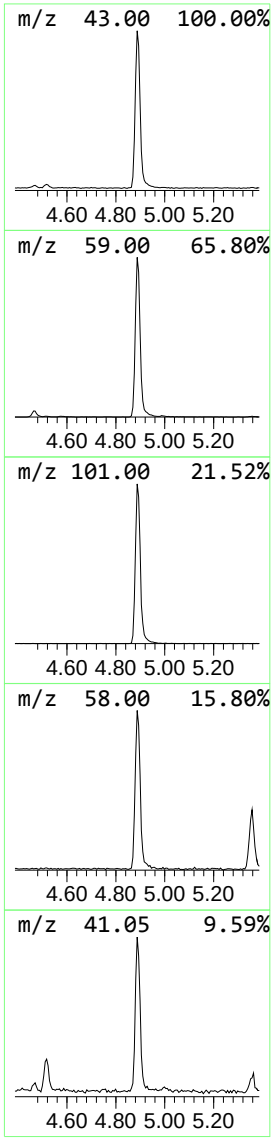
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	17.28 ng	462062	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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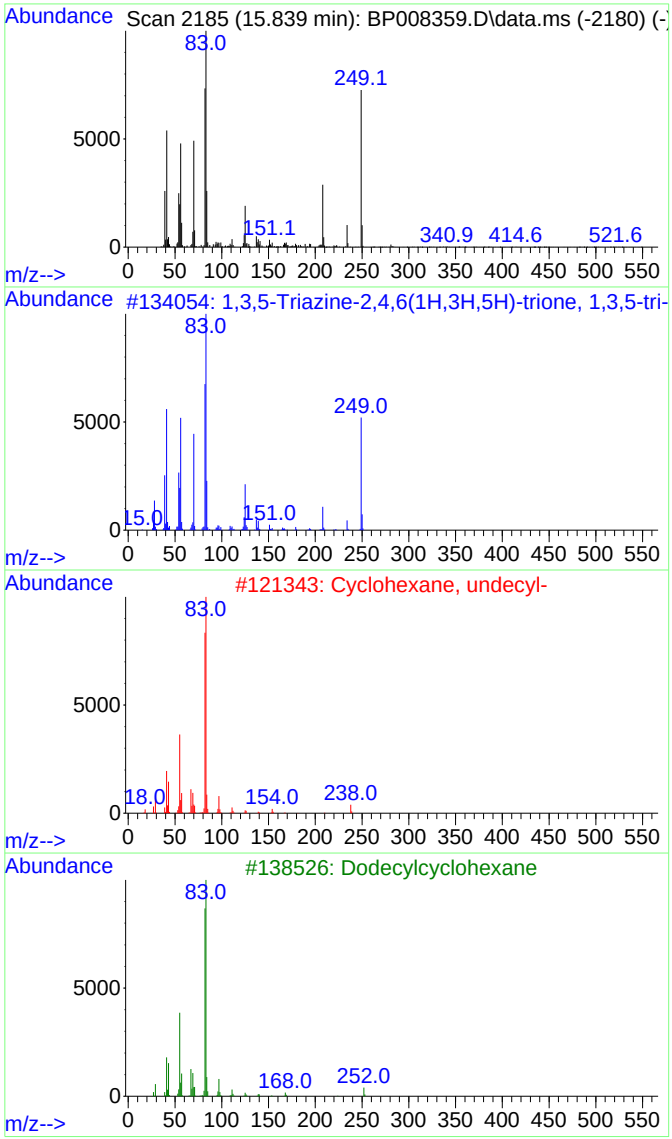
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

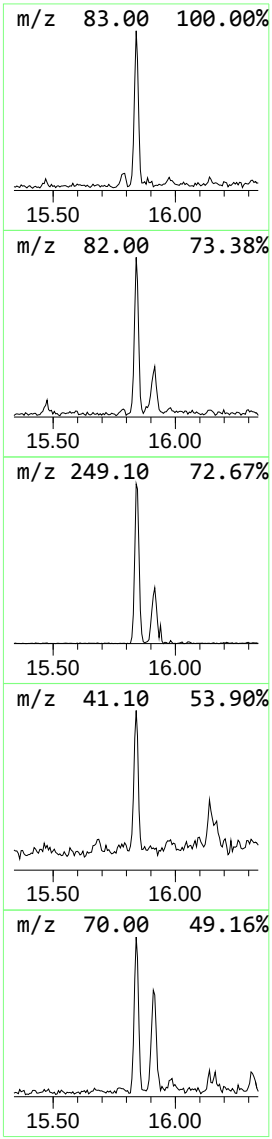
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	2.36 ng	98017	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	96
2	Cyclohexane, undecyl-	238	C17H34	054105-66-7	35
3	Dodecylcyclohexane	252	C18H36	001795-17-1	25
4	n-Pentadecylcyclohexane	294	C21H42	006006-95-7	25
5	Succinic acid, dec-2-yl trans-he...	340	C20H36O4	1000391-12-0	25





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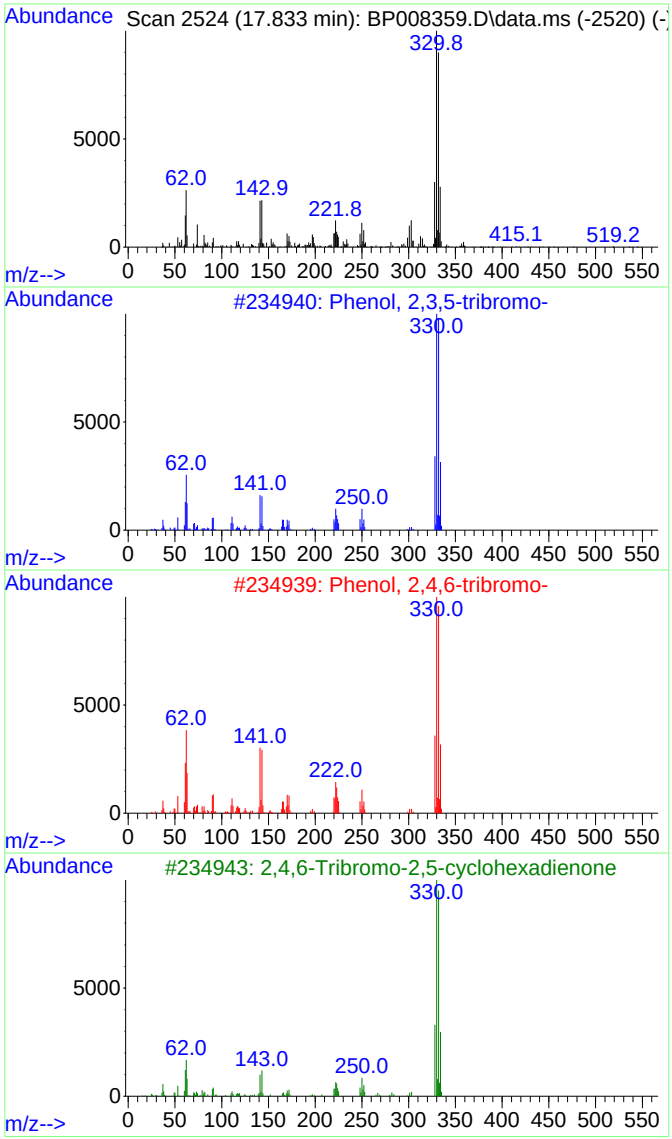
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

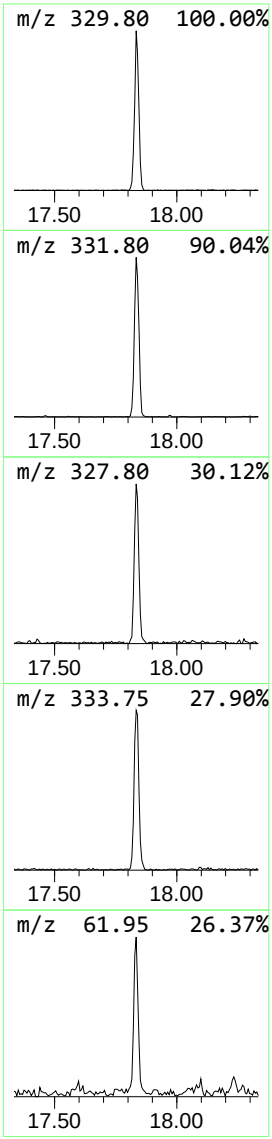
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 2,3,5-tribromo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.833	2.37 ng	98640	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	99
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	99
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	96
4	2,4,5-Tribromophenol	328	C6H3Br3O	014401-61-7	93
5	3,4,5-Tribromophenol	328	C6H3Br3O	116434-90-3	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

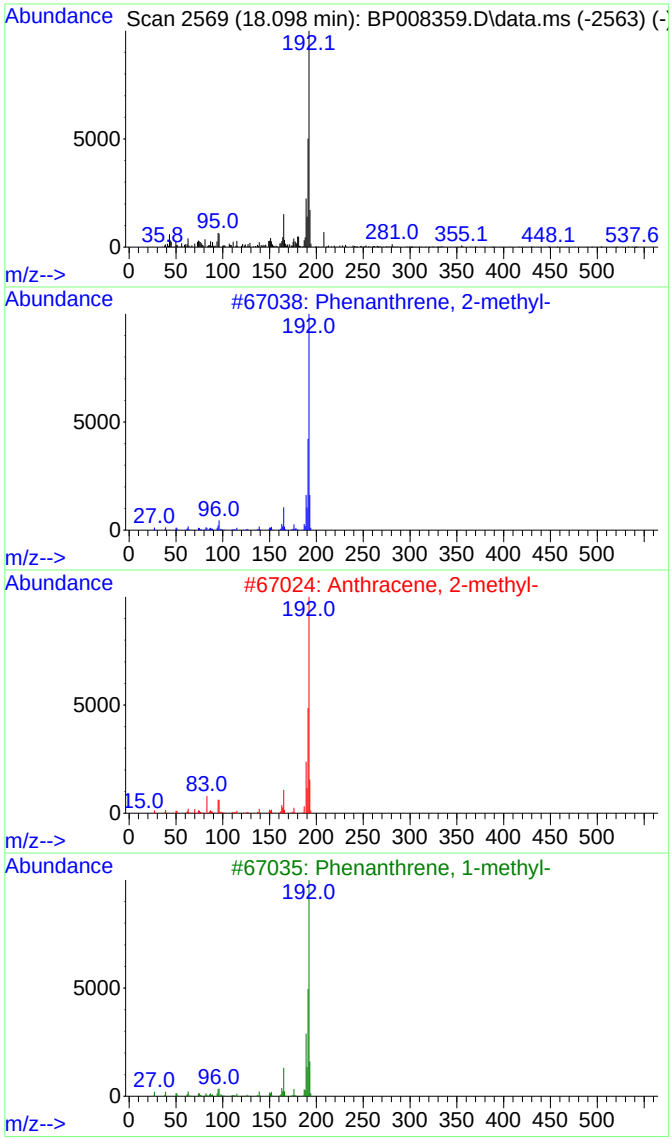
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

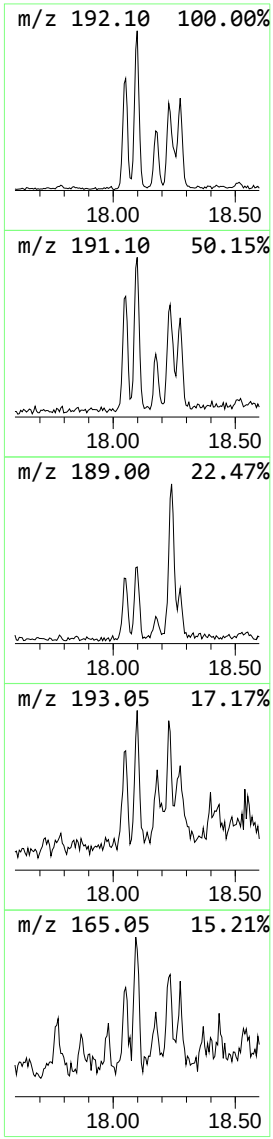
****

Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.36 ng	97971	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





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ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
R3-COMP

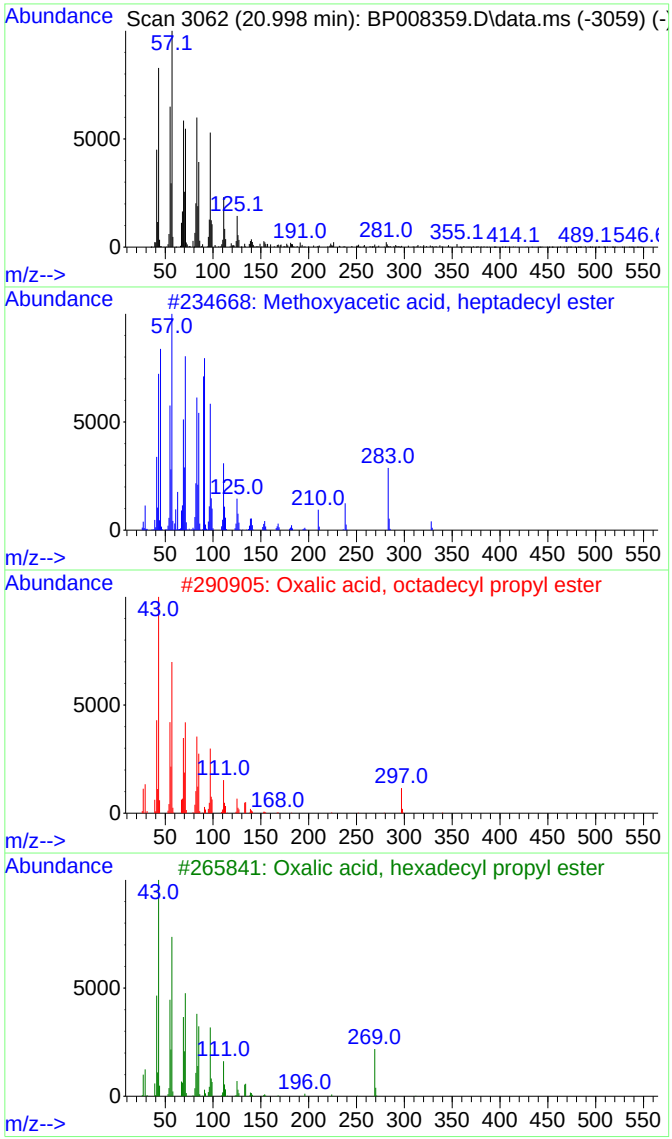
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

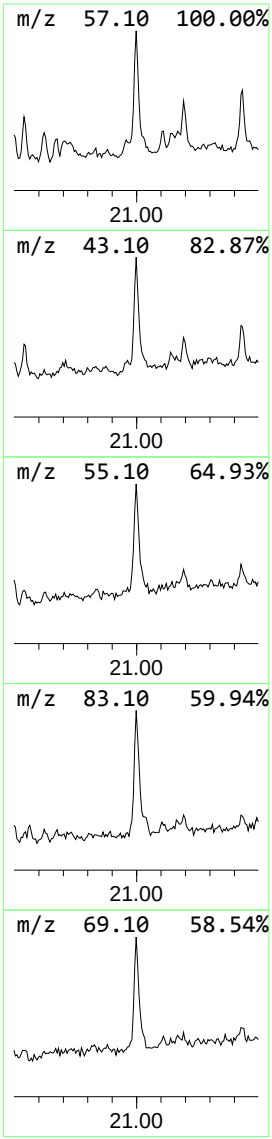
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Methoxyacetic acid, heptade... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	6.39 ng	411875	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	91
2	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	91
3	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121021\
Data File : BP008359.D
Acq On : 11 Dec 2021 01:37
Operator : CG/JU
Sample : M4990-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R3-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Furan, tetrahyd...	3.022	9.1	ng	242448	1	7.757	534651	20.0
3-Penten-2-one,...	4.293	2.1	ng	56701	1	7.757	534651	20.0
2-Pentanone, 4-...	4.887	17.3	ng	462062	1	7.757	534651	20.0
1,3,5-Triazine-...	15.839	2.4	ng	98017	4	17.175	831384	20.0
Phenol, 2,3,5-t...	17.833	2.4	ng	98640	4	17.175	831384	20.0
Phenanthrene, 2...	18.098	2.4	ng	97971	4	17.175	831384	20.0
Methoxyacetic a...	20.998	6.4	ng	411875	5	21.280	1288120	20.0