LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009197.D
Acq On : 17 Feb 2022 16:09
Operator : CG/JU
Sample : N1575-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

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-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.699	117	121	134	rVB	179778	253464	1.44%	0.370%
2	4.263	212	217	220	rBV	161307	237621	1.35%	0.347%
3	4.305	220	224	238	rVV	418732	658814	3.75%	0.961%
4	4.416	238	243	253	rVB	200287	282701	1.61%	0.412%
5	4.899	320	325	338	rBV	279444	467817	2.66%	0.682%
6	5.375	399	406	436	rBV	2427973	4381841	24.92%	6.390%
7	6.969	671	677	710	rVB	1610884	3352688	19.07%	4.889%
8	7.334	733	739	743	rBV	108841	180551	1.03%	0.263%
9	7.387	743	748	757	rVB	104092	199082	1.13%	0.290%
10	7.575	774	780	798	rBV	156645	345492	1.97%	0.504%
11	7.775	806	814	822	rBV	720494	1235247	7.03%	1.801%
12	8.940	1005	1012	1040	rBV	2258032	4345754	24.72%	6.337%
13	10.575	1279	1290	1308	rBV	823129	1710988	9.73%	2.495%
14	13.039	1702	1709	1735	rBV	7510158	12142912	69.07%	17.707%
15	13.275	1739	1749	1763	rBV	387721	743544	4.23%	1.084%
16	14.322	1919	1927	1937	rBV3	70378	225958	1.29%	0.329%
17	14.422	1937	1944	1957	rVB	1507014	2524301	14.36%	3.681%
18	15.245	2077	2084	2096	rVB2	94812	195620	1.11%	0.285%
19	15.922	2192	2199	2217	rBV	5741369	9579643	54.49%	13.969%
20	17.180	2407	2413	2431	rBV	1904122	3163596	17.99%	4.613%
21	18.080	2562	2566	2575	rBV3	81310	182257	1.04%	0.266%
22	19.745	2843	2849	2866	rBV	14196774	17581443	100.00%	25.637%
23	21.063	3069	3073	3080	rBV	185519	327963	1.87%	0.478%
24	21.280	3105	3110	3121	rBV	2059946	3125364	17.78%	4.557%
25	23.680	3513	3518	3532	rVB3	412244	1132444	6.44%	1.651%

Sum of corrected areas: 68577105

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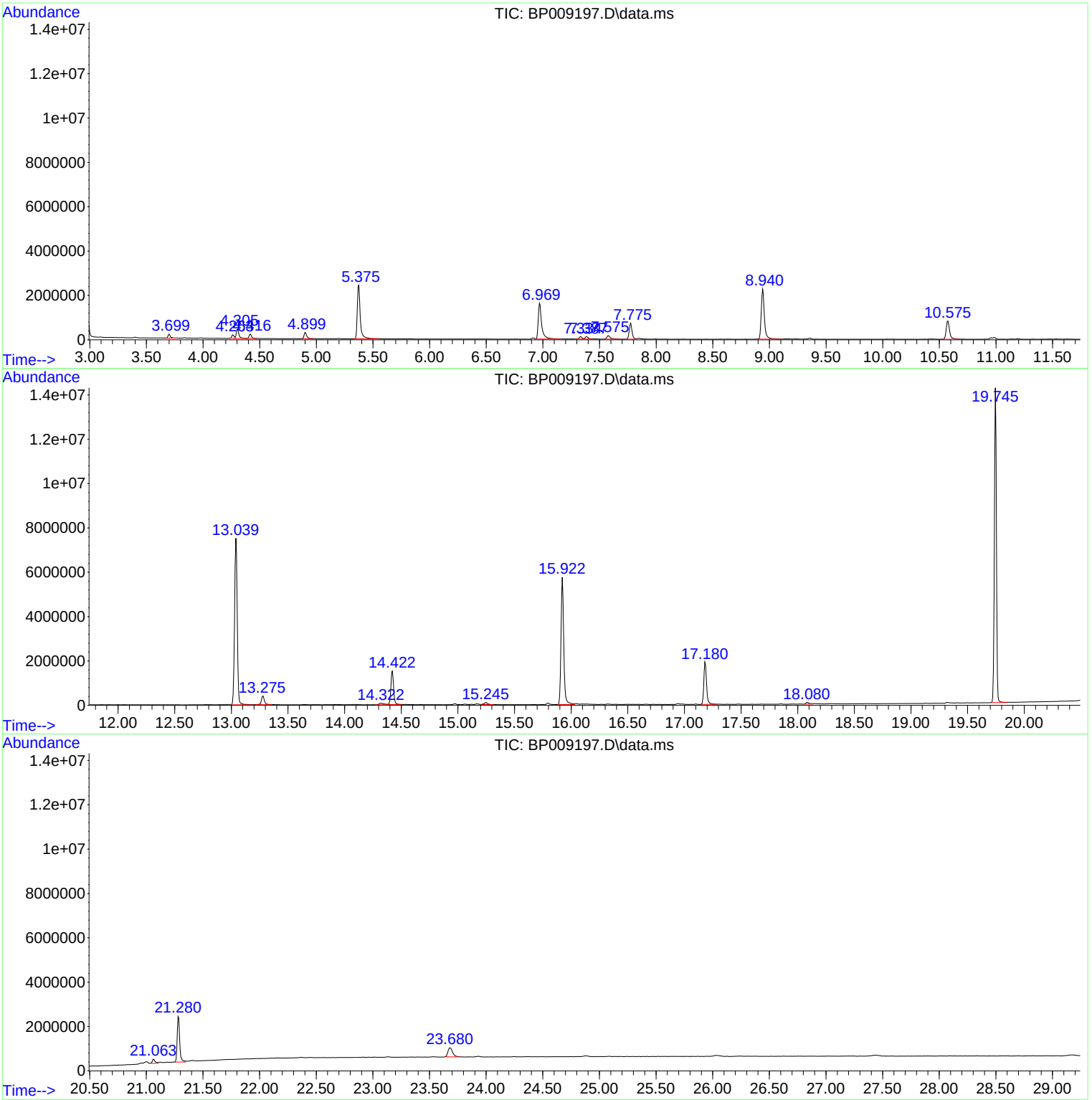
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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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Data File : BP009197.D
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TIC Library : C:\Database\NIST20.L
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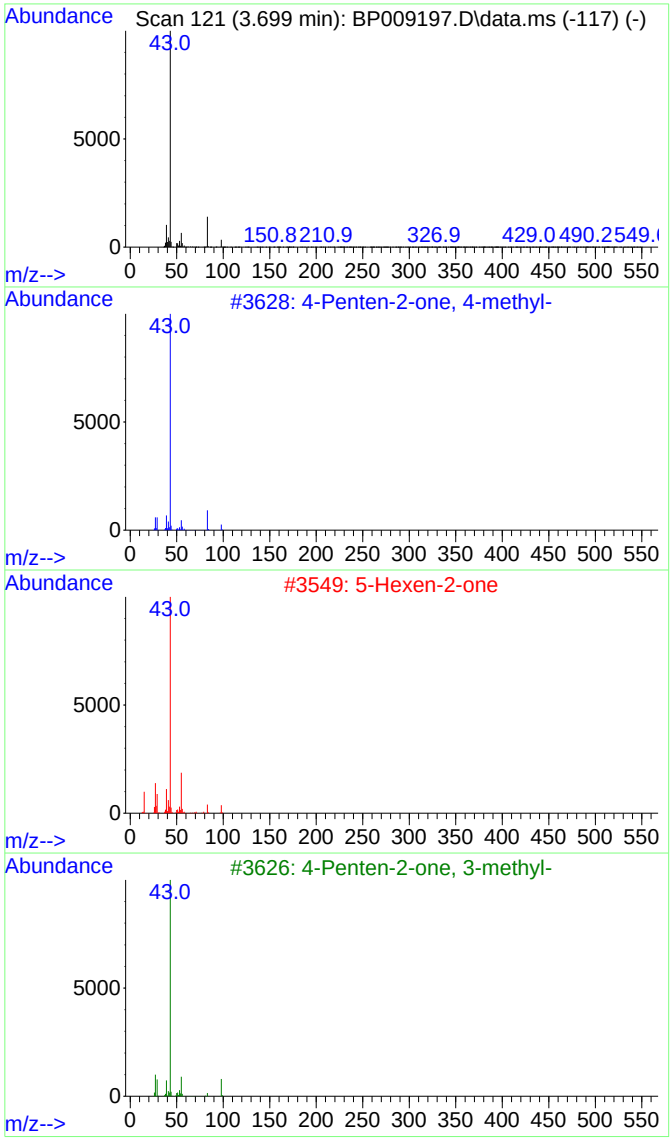
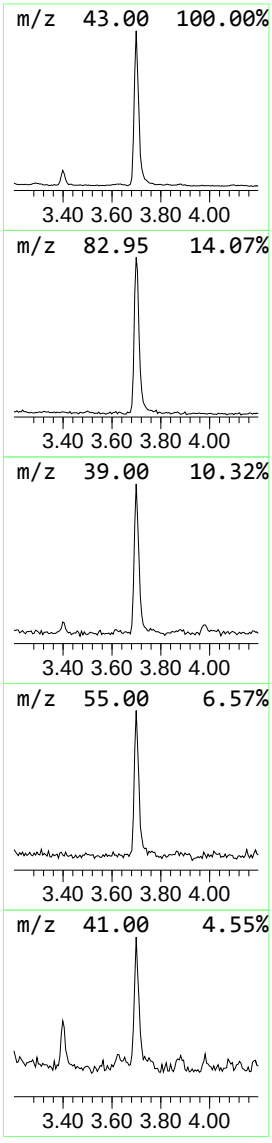
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.699	4.10 ng	253464	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
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-Vinylethyl acetate	114	C6H10O2	001576-84-7	40
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17





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Data File : BP009197.D
Acq On : 17 Feb 2022 16:09
Operator : CG/JU
Sample : N1575-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

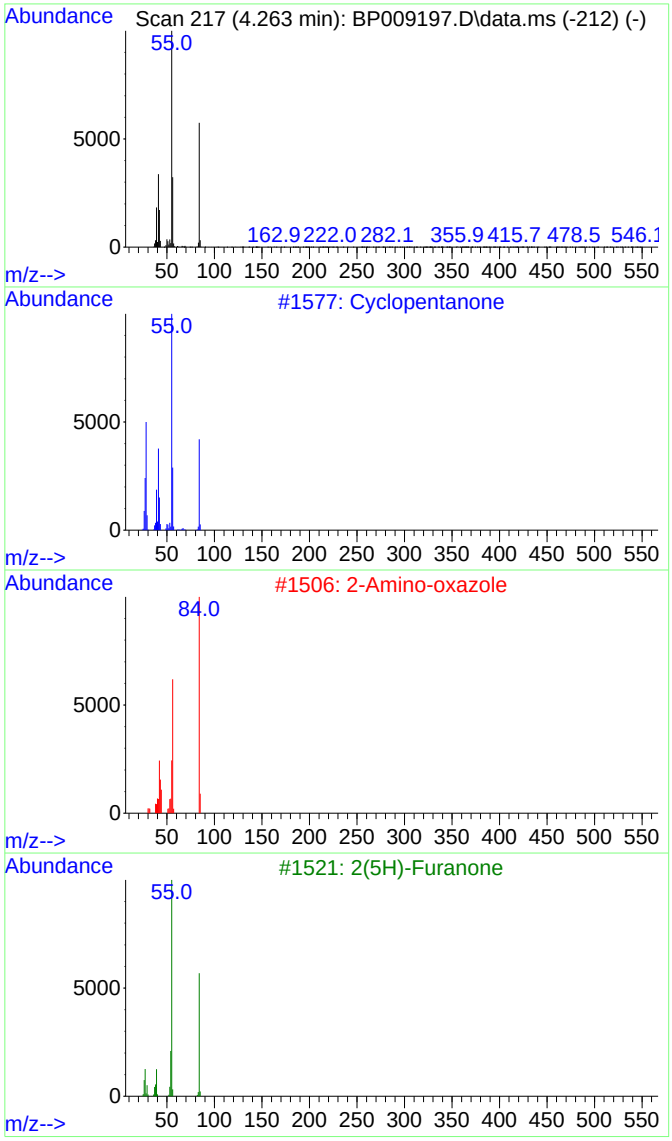
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

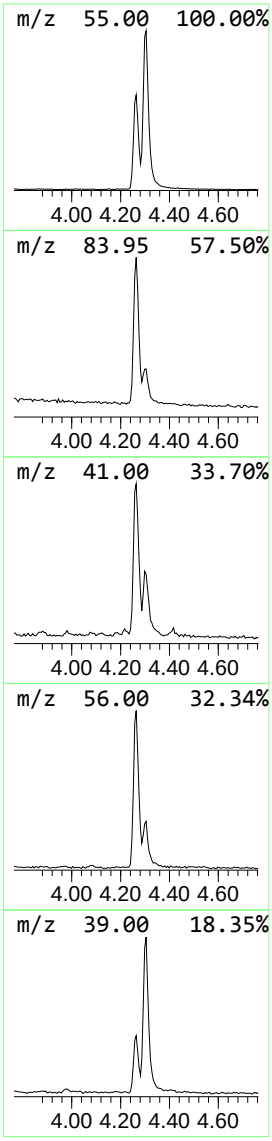
****

Peak Number 2 Cyclopentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.263	3.85 ng	237621	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Amino-oxazole	84	C3H4N2O	004570-45-0	53
3	2(5H)-Furanone	84	C4H4O2	000497-23-4	52
4	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	45
5	3-Hexene	84	C6H12	000592-47-2	40





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Acq On : 17 Feb 2022 16:09
Operator : CG/JU
Sample : N1575-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

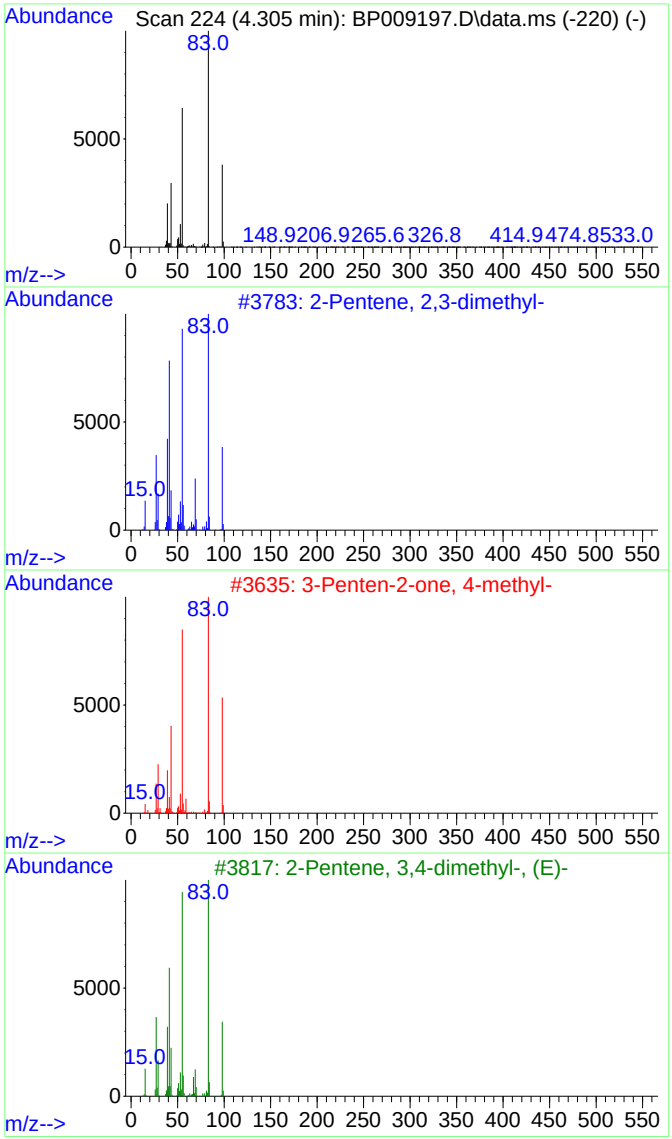
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

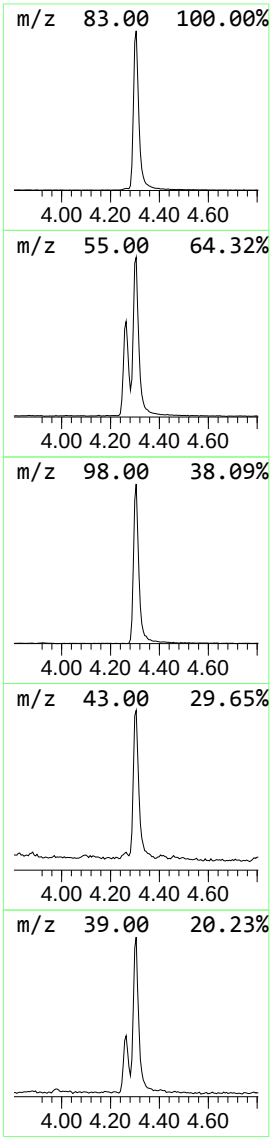
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentene, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.305	10.67 ng	658814	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
4	3-Hexen-2-one	98	C6H10O	000763-93-9	83
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





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Instrument :
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ClientSampleId :
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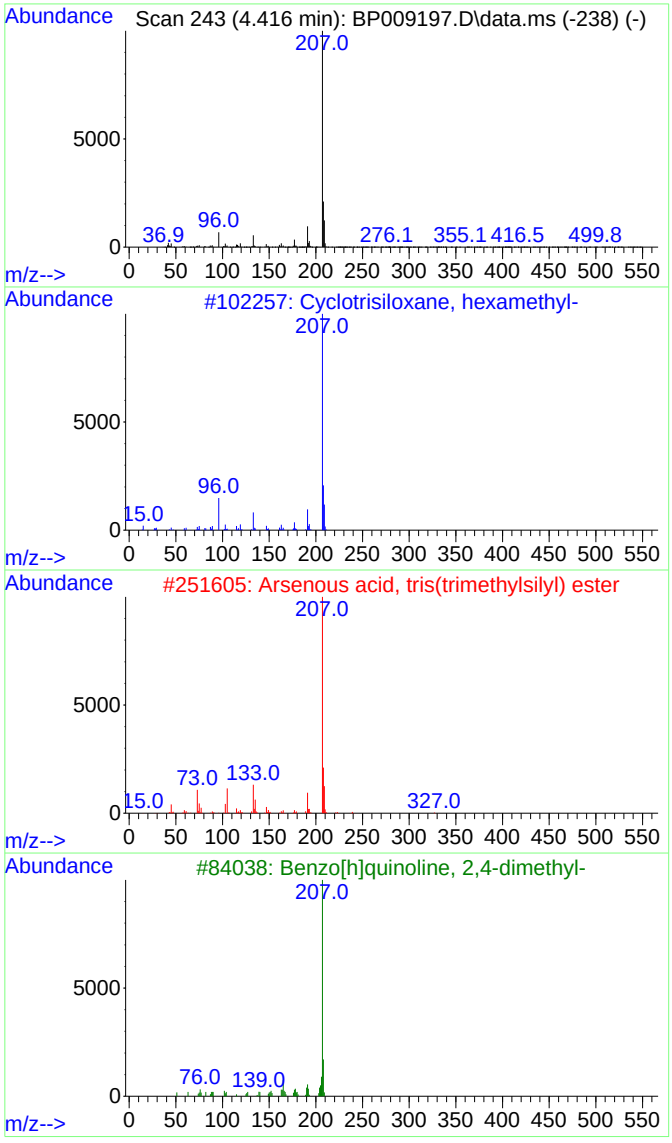
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

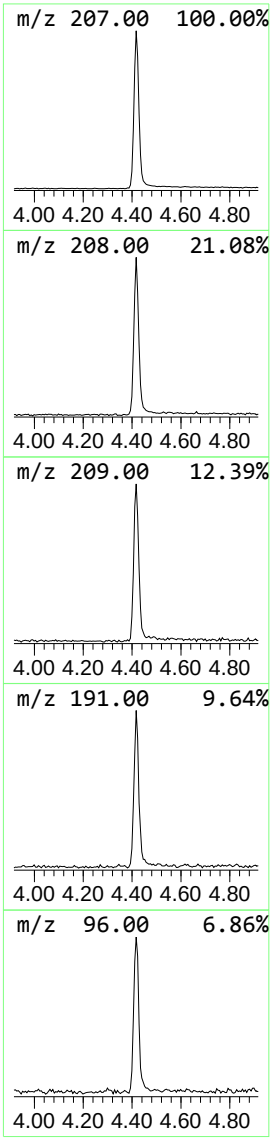
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	4.58 ng	282701	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	90
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	78
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	45
4	4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	39
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39





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Sample : N1575-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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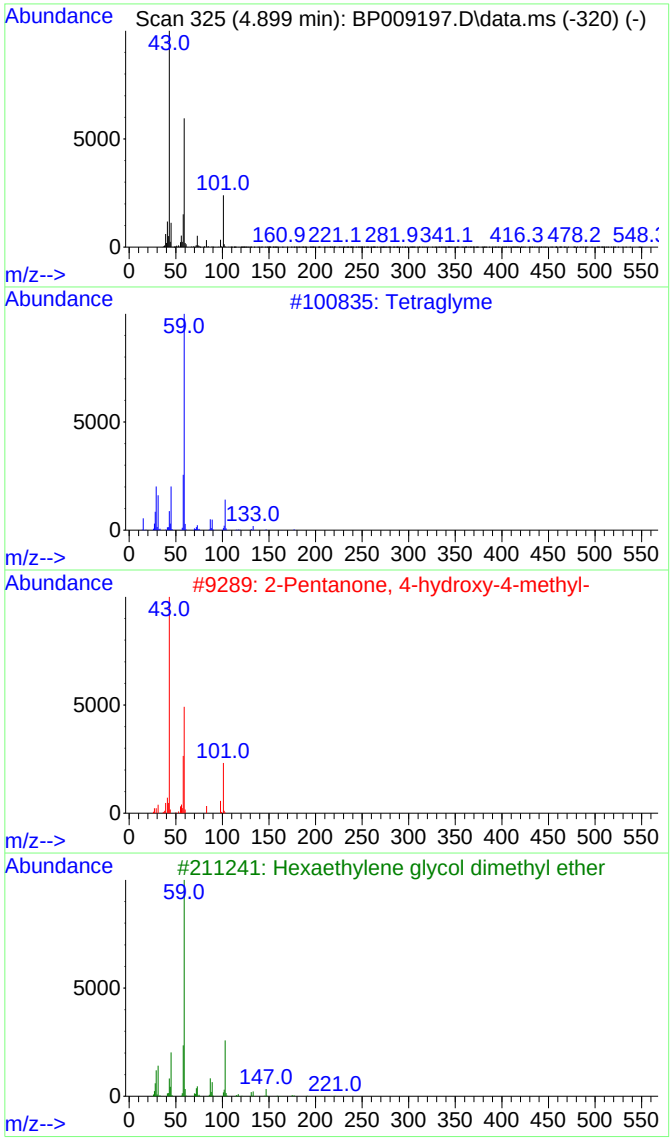
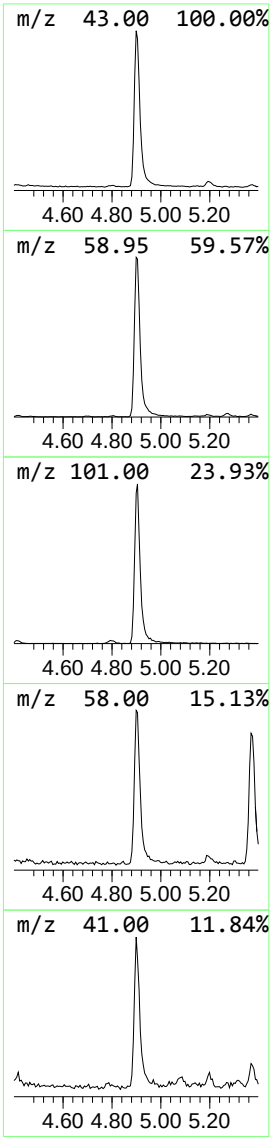
****

Peak Number 5 unknown4.899 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	7.57 ng	467817	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetraglyme	222	C10H22O5	000143-24-8	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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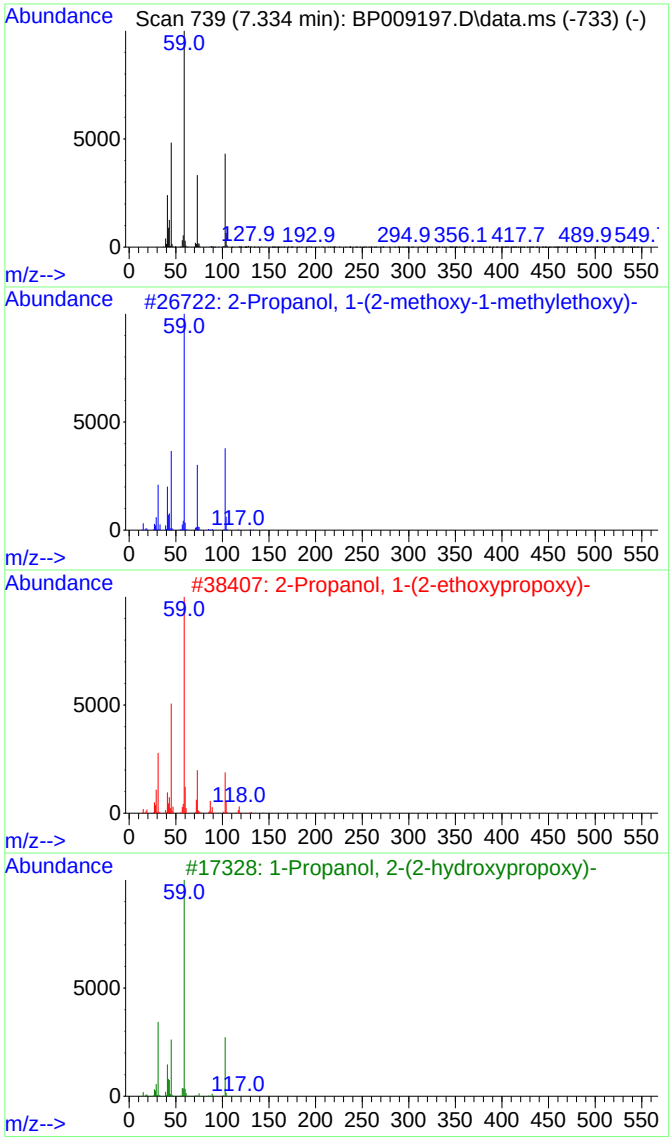
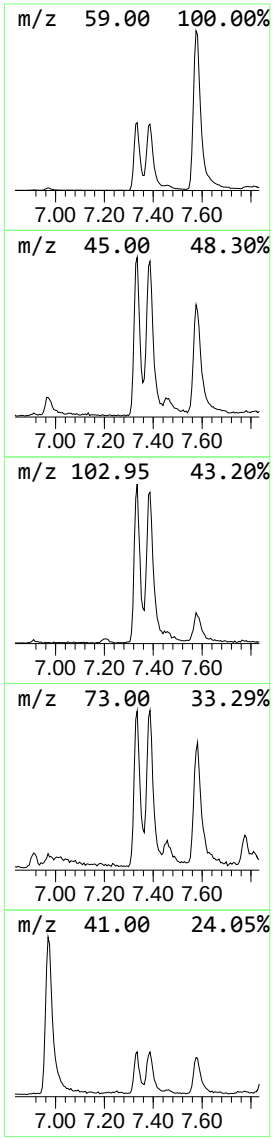
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.334	2.92 ng	180551	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	43
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	42
5	Ethyl 2,5,8,11-tetraoxatridecan-...	250	C11H22O6	1000366-77-9	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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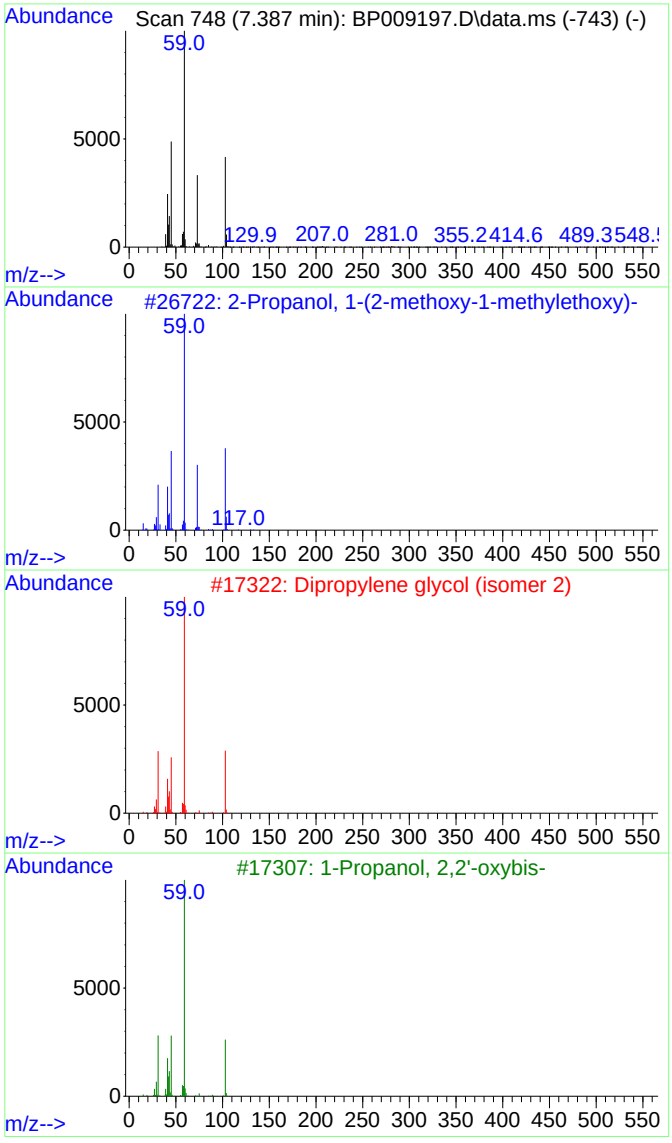
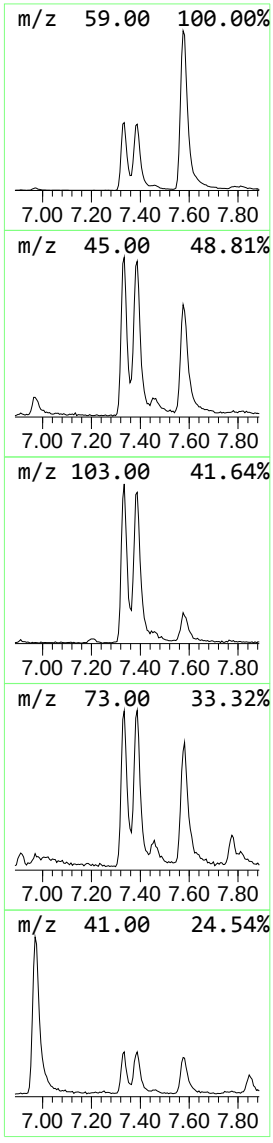
****

Peak Number 7 Dipropylene glycol (isomer 2) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.387	3.22 ng	199082	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	59
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
5	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	53





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TIC Library : C:\Database\NIST20.L
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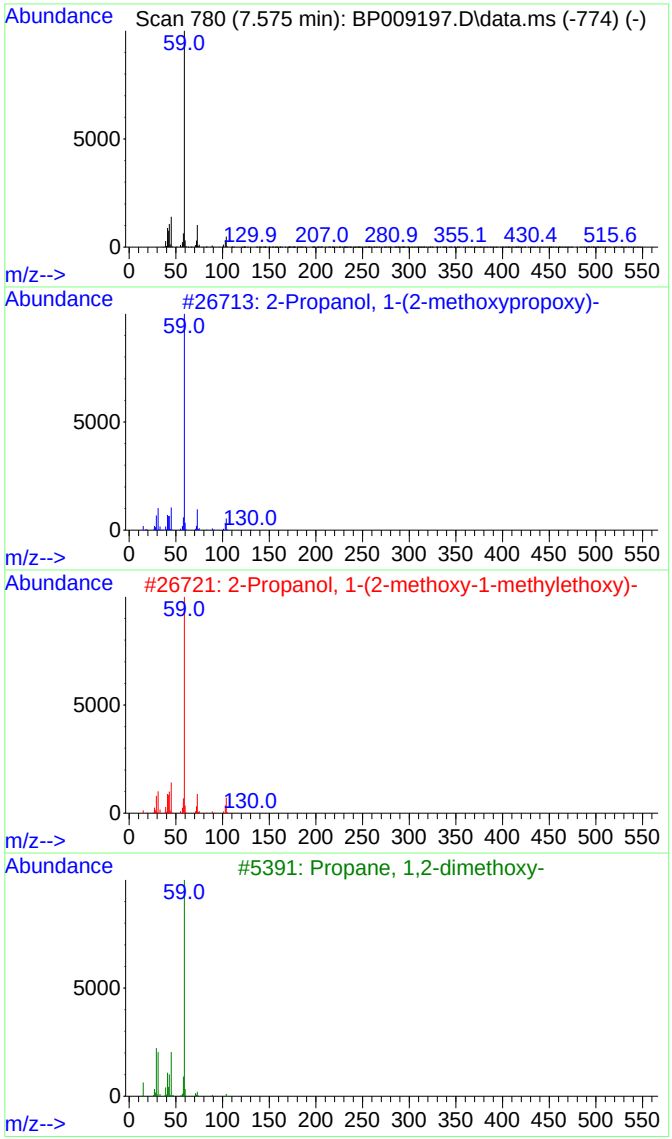
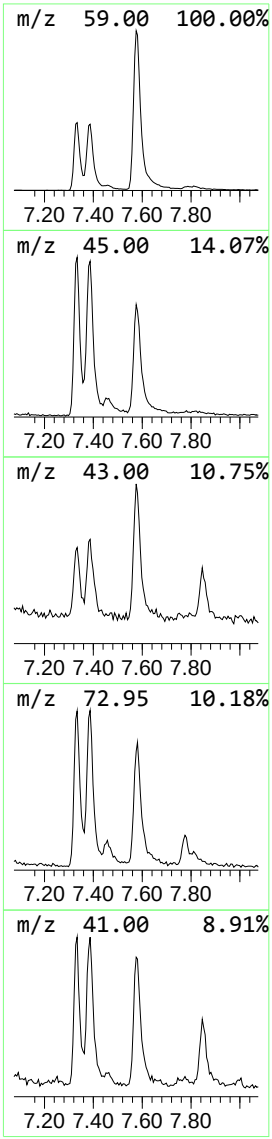
****

Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	5.59 ng	345492	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	72
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50





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BNA_P
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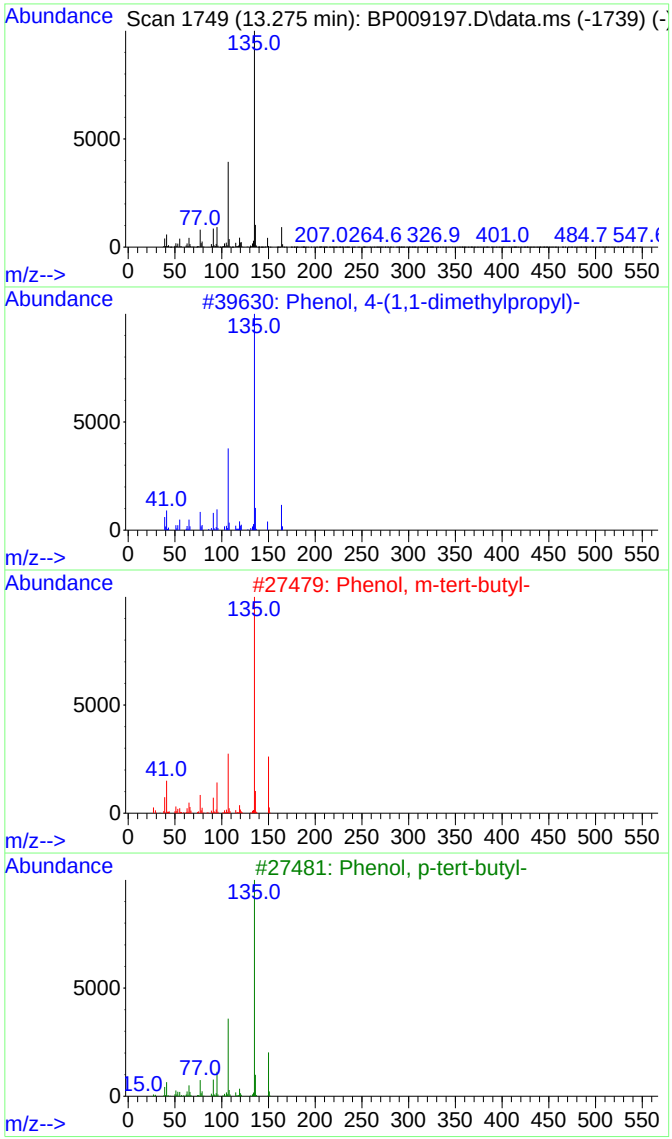
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

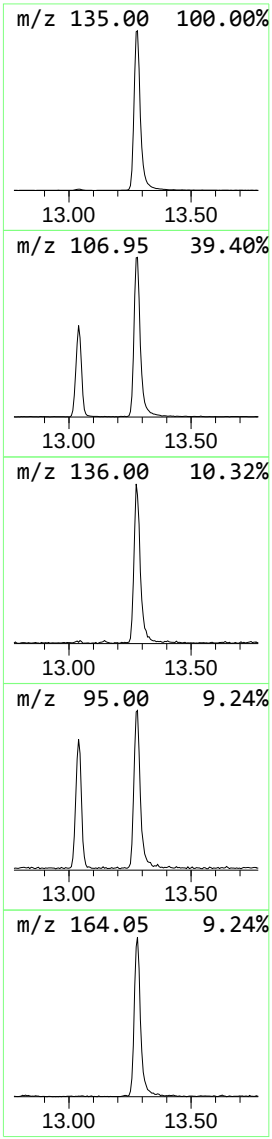
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.275	5.89 ng	743544	Acenaphthene-d10	14.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	97
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

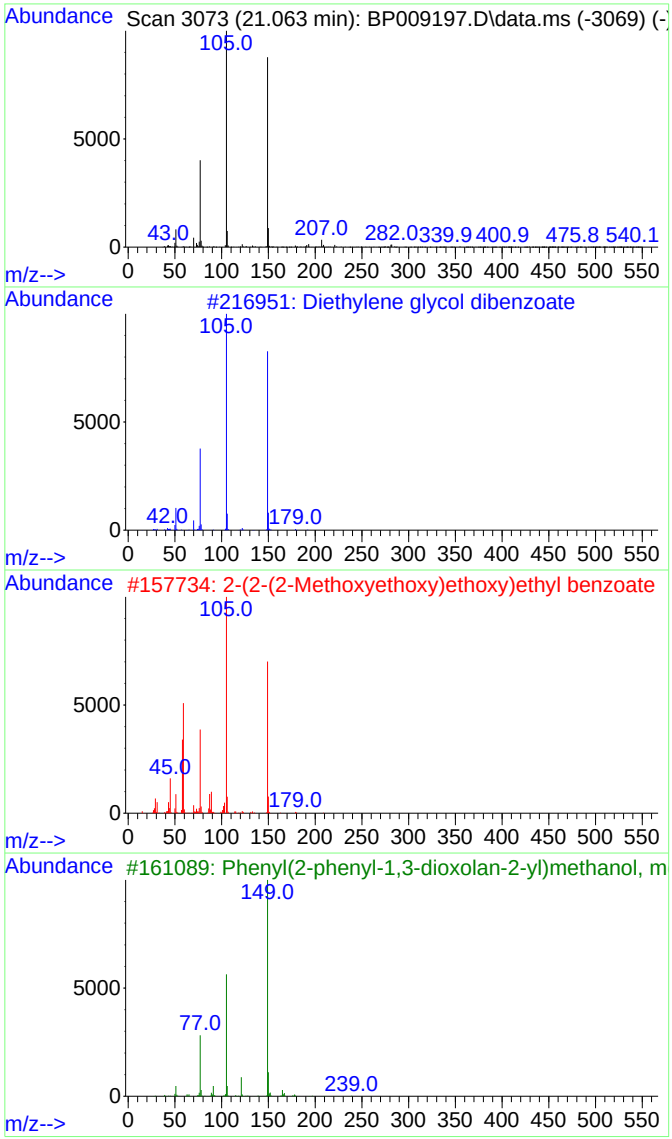
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

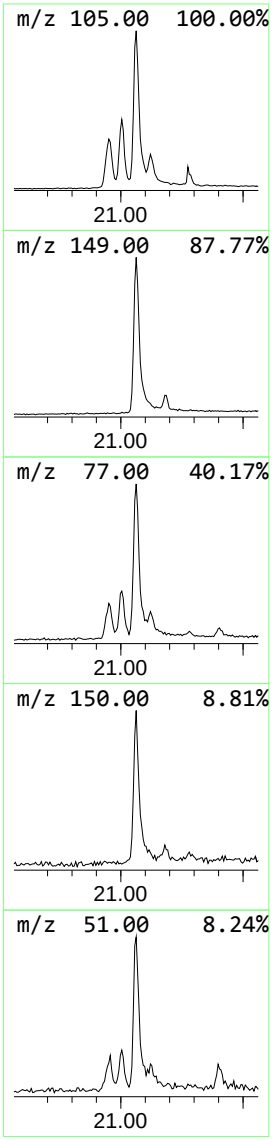
****

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	2.10 ng	327963	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	87
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	78
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64
5	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009197.D
Acq On : 17 Feb 2022 16:09
Operator : CG/JU
Sample : N1575-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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
4-Penten-2-one,...	3.699	4.1	ng	253464	1	7.775	1235250	20.0
Cyclopentanone	4.263	3.9	ng	237621	1	7.775	1235250	20.0
2-Pentene, 2,3-...	4.305	10.7	ng	658814	1	7.775	1235250	20.0
Cyclotrisiloxan...	4.416	4.6	ng	282701	1	7.775	1235250	20.0
unknown4.899	4.899	7.6	ng	467817	1	7.775	1235250	20.0
2-Propanol, 1-(...	7.334	2.9	ng	180551	1	7.775	1235250	20.0
Dipropylene gly...	7.387	3.2	ng	199082	1	7.775	1235250	20.0
2-Propanol, 1-(...	7.575	5.6	ng	345492	1	7.775	1235250	20.0
Phenol, 4-(1,1-...	13.275	5.9	ng	743544	3	14.422	2524300	20.0
Diethylene glyc...	21.063	2.1	ng	327963	5	21.280	3125360	20.0