LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005419.D
Acq On : 29 Apr 2021 20:39
Operator : CG/JU
Sample : M2202-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 290

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-BP042921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005419.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.175	179	185	190	rBV2	24400	34020	1.88%	0.375%
2	4.775	278	287	296	rBV	842919	1087941	60.06%	11.996%
3	5.228	359	364	375	rVB	92013	137378	7.58%	1.515%
4	6.816	627	634	647	rBV	280632	468905	25.89%	5.170%
5	7.622	765	771	780	rBV	123710	199754	11.03%	2.203%
6	8.787	962	969	987	rBV	403750	653755	36.09%	7.208%
7	10.416	1237	1246	1254	rBV	140941	244199	13.48%	2.693%
8	12.904	1662	1669	1688	rBV	856274	1227365	67.76%	13.533%
9	13.757	1808	1814	1822	rBV	31814	47673	2.63%	0.526%
10	14.293	1895	1905	1913	rBV2	228647	341778	18.87%	3.769%
11	15.798	2155	2161	2170	rBV2	72302	112111	6.19%	1.236%
12	17.057	2369	2375	2385	rBV	312991	444733	24.55%	4.904%
13	17.963	2524	2529	2536	rBV3	18939	35804	1.98%	0.395%
14	19.639	2808	2814	2820	rBV	1565900	1811297	100.00%	19.972%
15	20.845	3013	3019	3022	rBV	81007	137348	7.58%	1.514%
16	20.892	3023	3027	3032	rVV	126893	186862	10.32%	2.060%
17	20.945	3032	3036	3045	rVV	464921	590188	32.58%	6.508%
18	21.010	3045	3047	3052	rVB	27326	32937	1.82%	0.363%
19	21.163	3068	3073	3077	rBV	520376	633418	34.97%	6.984%
20	23.410	3449	3455	3464	rVB2	355772	641847	35.44%	7.077%

Sum of corrected areas: 9069313

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Misc :
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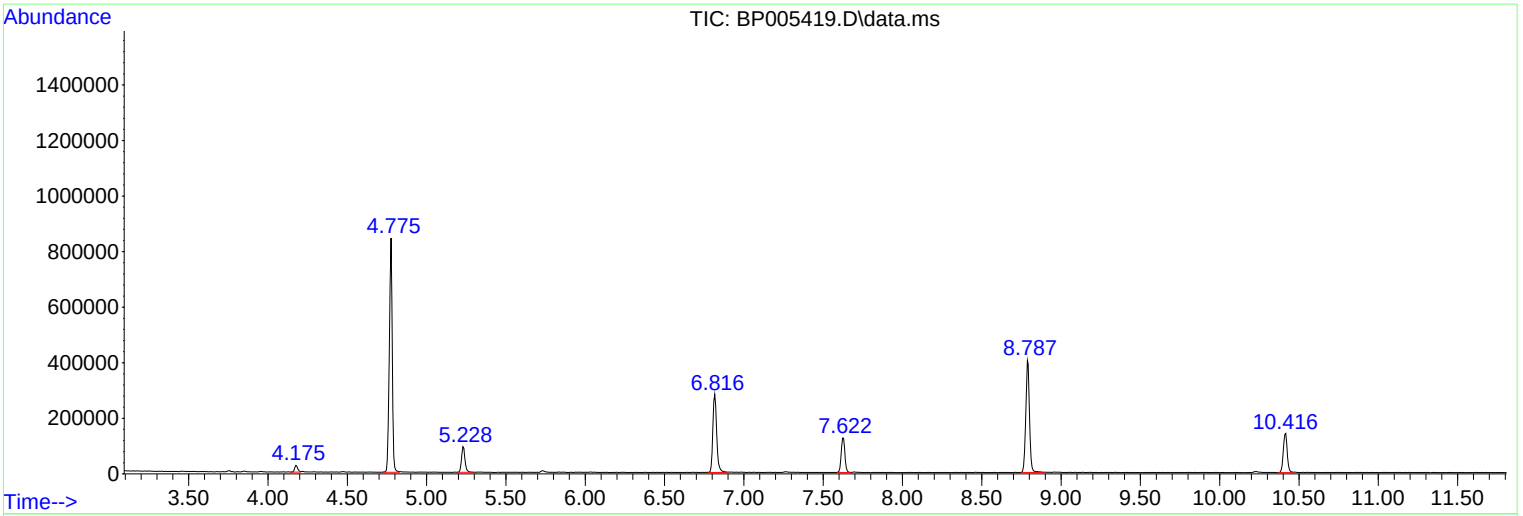
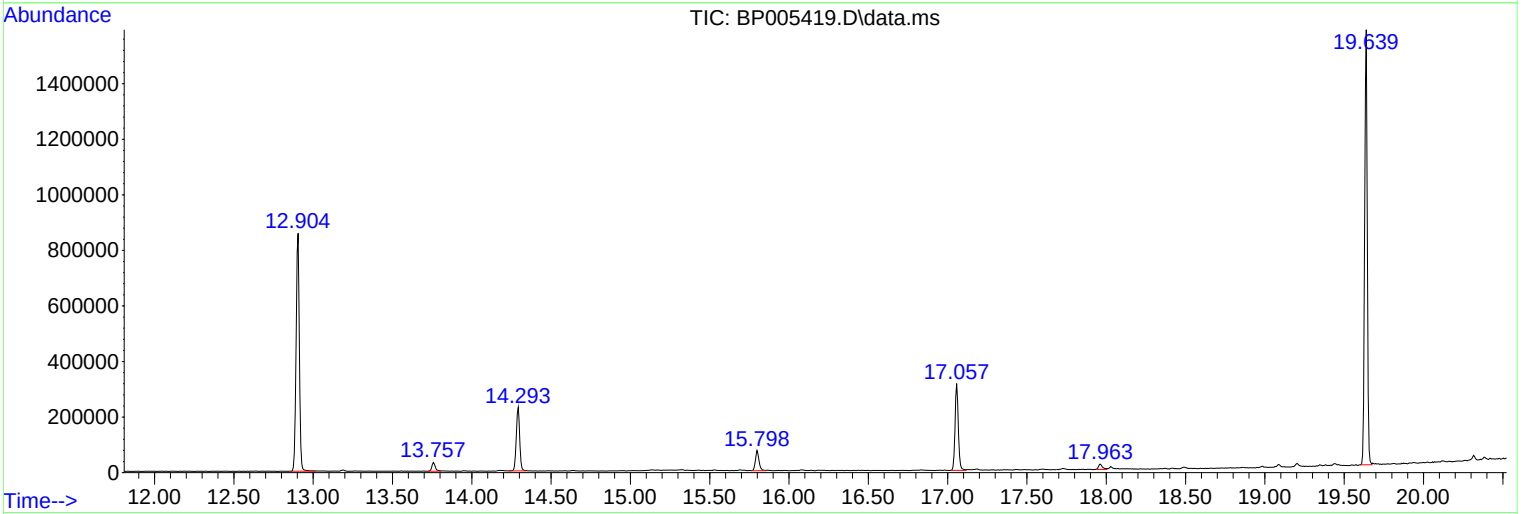
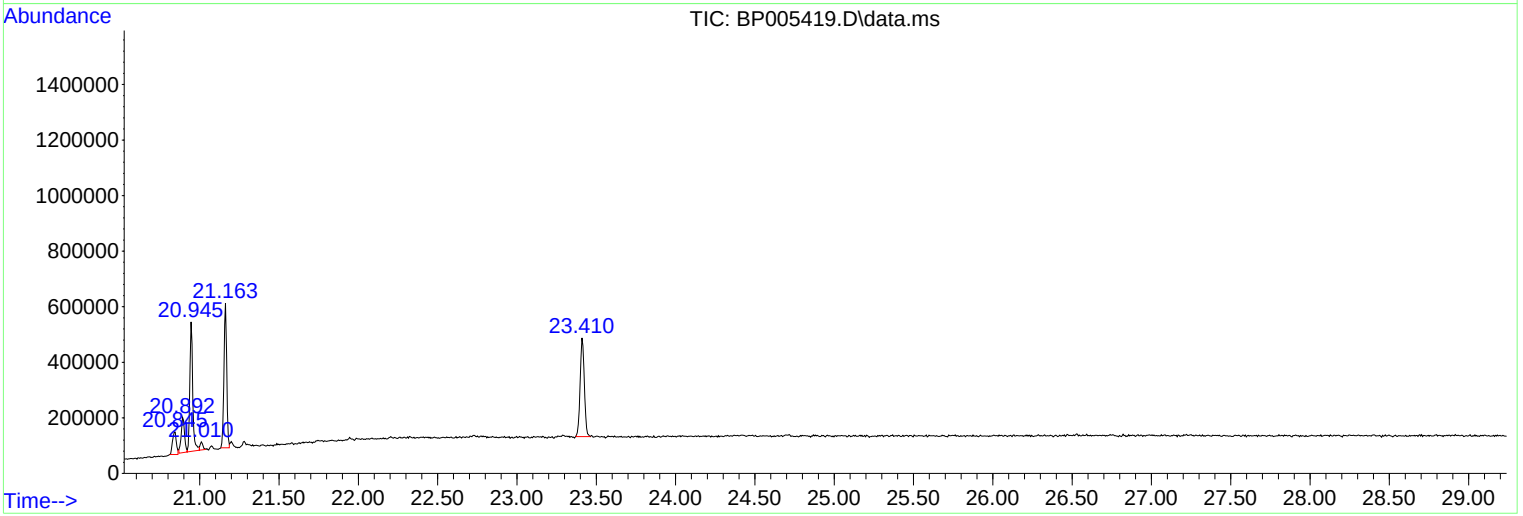
Instrument :
BNA_P
ClientSampleId :
290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.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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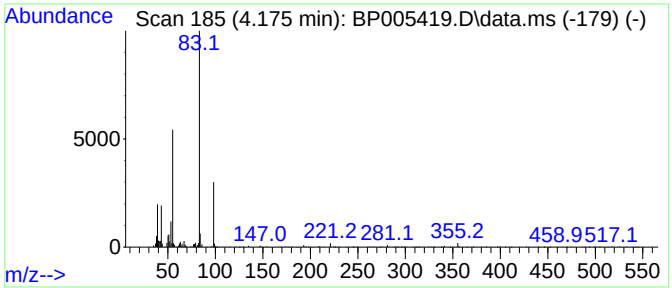
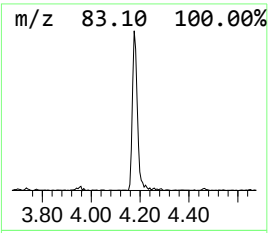
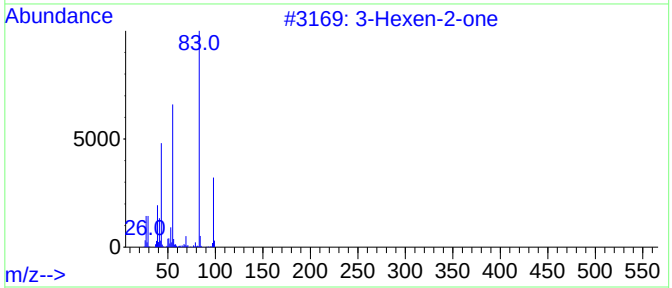
Peak Number 1 3-Hexen-2-one Concentration Rank 5

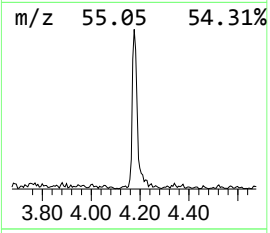
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.175	3.41 ng	34020	1,4-Dichlorobenzene-d4	7.628

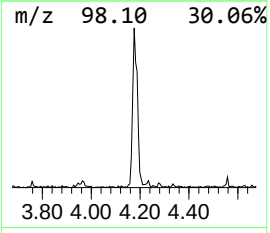
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	86
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	64
3	Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	59
4	1,5-Heptadien-4-one, 3,3,6-trime...	152	C10H16O	000546-49-6	59
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	56

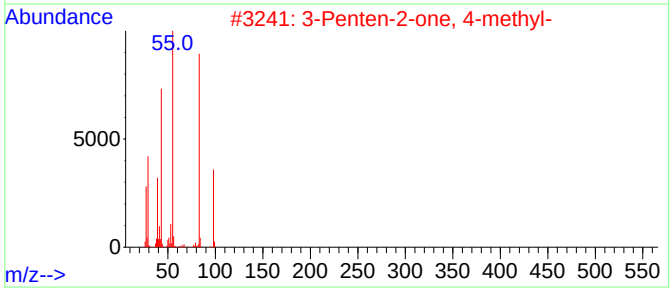


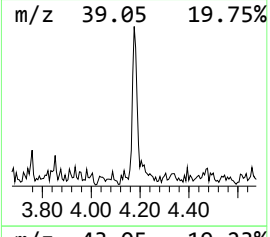


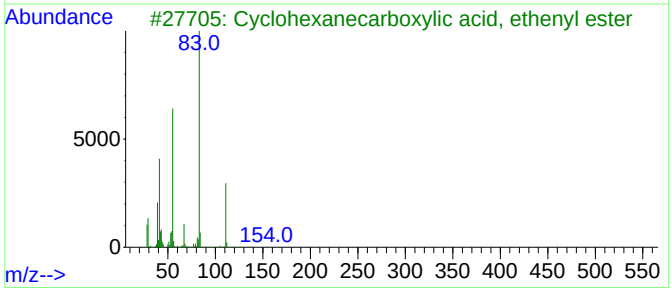


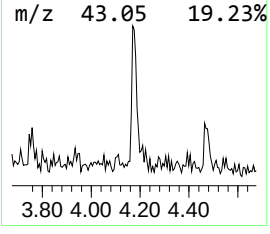












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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

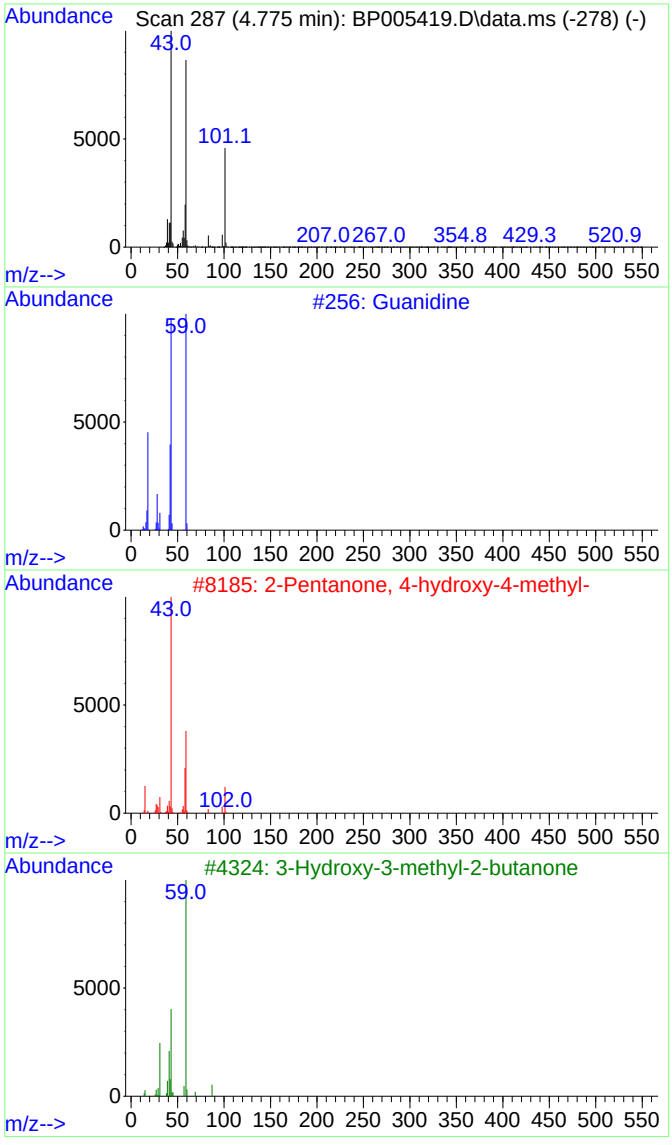
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

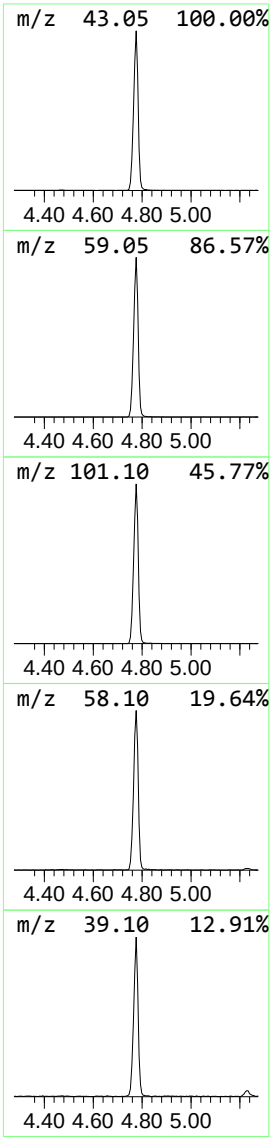
****

Peak Number 2 unknown4.775 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.775	108.93 ng	1087940	1,4-Dichlorobenzene-d4	7.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	38
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Instrument : BNA_P
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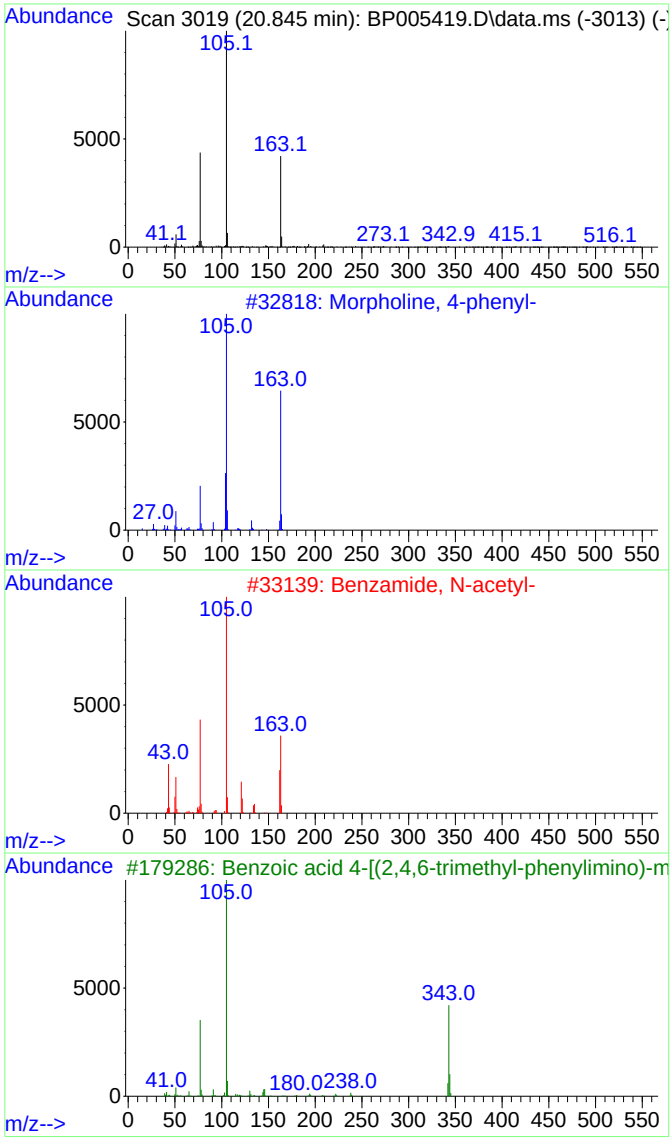
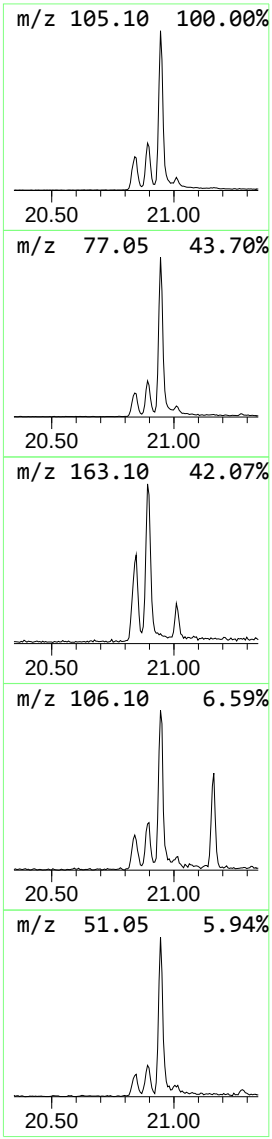
Peak Number 3 unknown20.845 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	4.34 ng	137348	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
2	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	40
3	Benzoic acid 4-[(2,4,6-trimethyl...	343	C23H21NO2	304448-58-6	23
4	Biphenyl, 4,4'-dibenzoyloxy-	394	C26H18O4	1000294-15-4	12
5	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	9





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Sample : M2202-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 290

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
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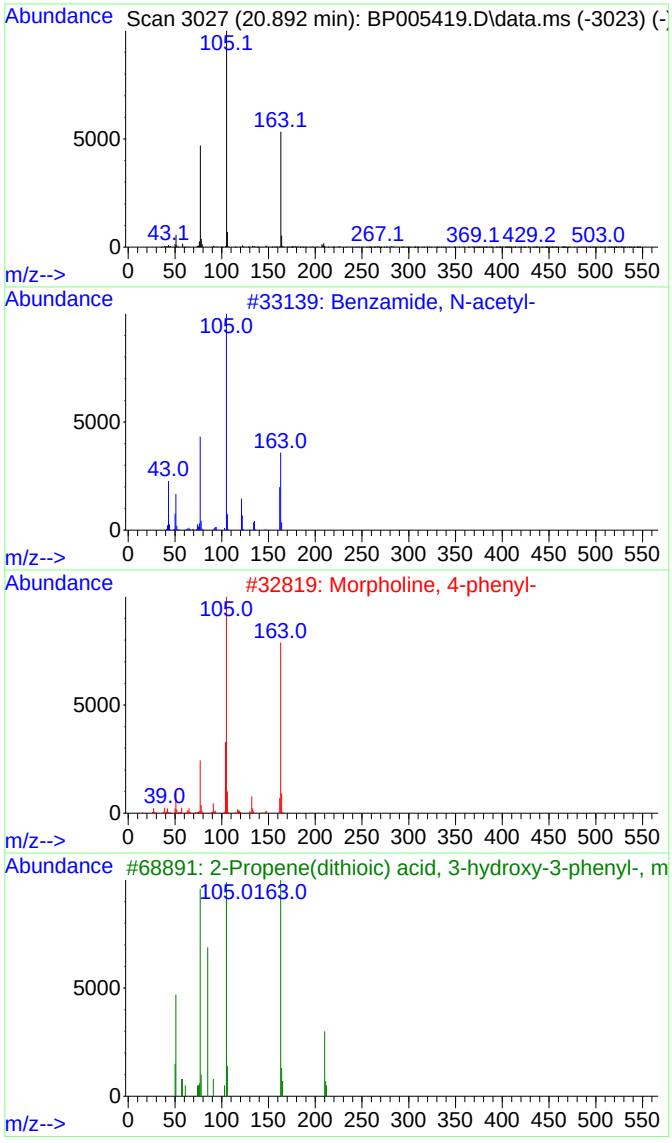
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

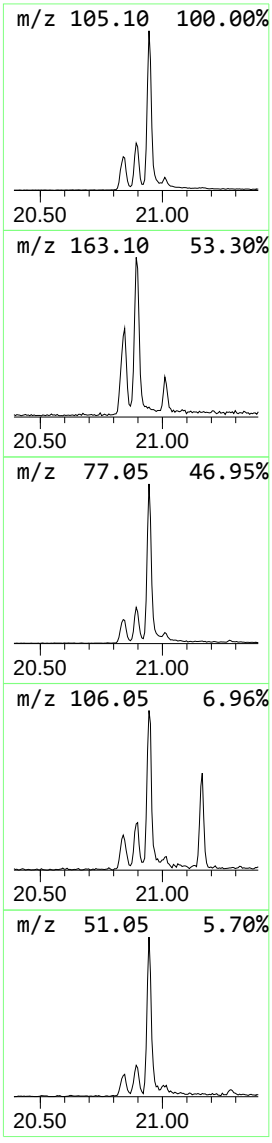
****

Peak Number 4 Benzamide, N-acetyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	5.90 ng	186862	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	78
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
3	2-Propene(dithioic) acid, 3-hydr...	210	C10H10OS2	013636-68-5	43
4	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	38
5	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	25





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Instrument : BNA_P
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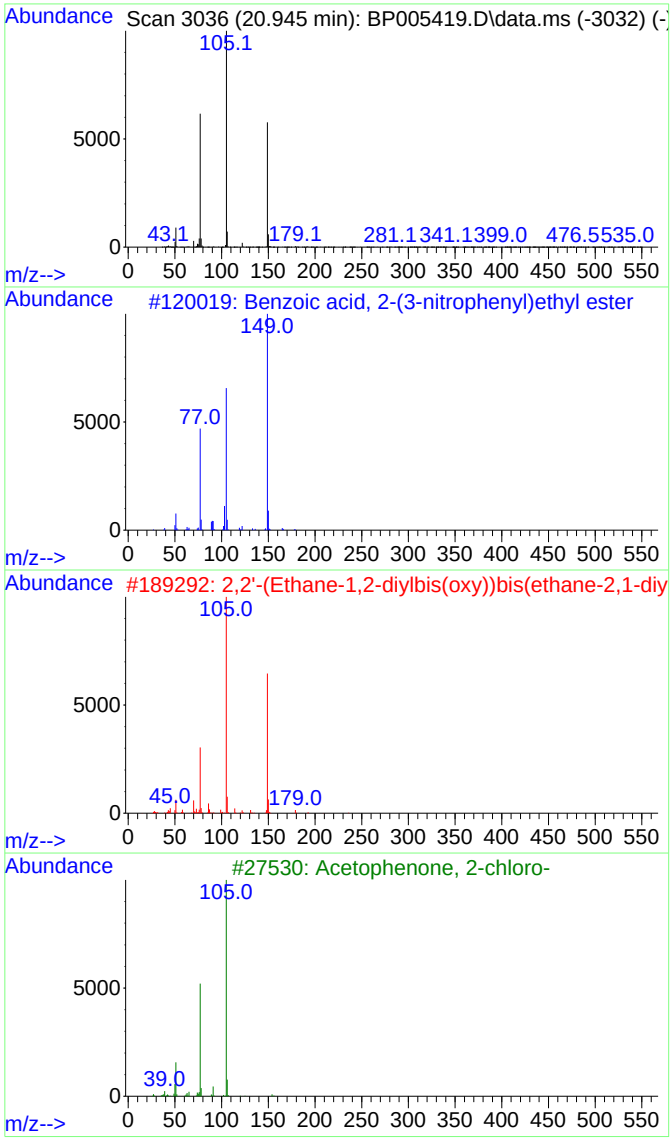
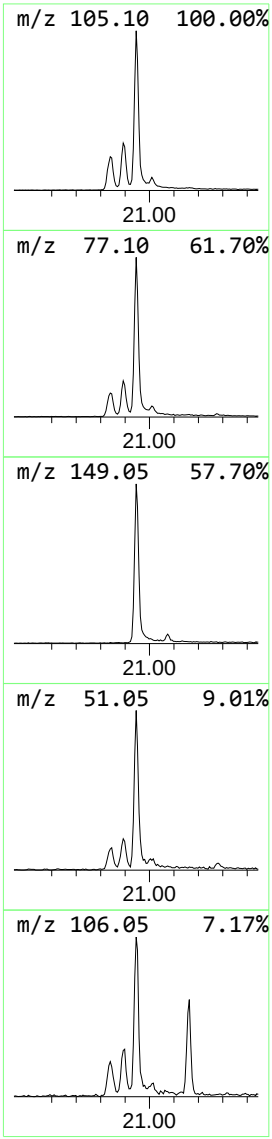
****
Peak Number 5 Benzoic acid, 2-(3-nitrophe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	18.64 ng	590188	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	45





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Hexen-2-one	4.175	3.4	ng	34020	1	7.628	199754	20.0
unknown4.775	4.775	108.9	ng	1087940	1	7.628	199754	20.0
unknown20.845	20.845	4.3	ng	137348	5	21.163	633418	20.0
Benzamide, N-ac...	20.892	5.9	ng	186862	5	21.163	633418	20.0
Benzoic acid, 2...	20.945	18.6	ng	590188	5	21.163	633418	20.0